

On the hyperfine anomaly and precision searches for new physics

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THE UNIVERSITY
OF QUEENSLAND
AUSTRALIA



Australian Government
Australian Research Council



INT-24-1 Fundamental Physics with Radioactive Molecules

Overview

Testing the SM and searching for new physics in atoms

- Atomic parity violation
- Time-reversal-violating electric dipole moments

Adventures at the intersection of atomic and nuclear physics

- Case study in the hyperfine structure

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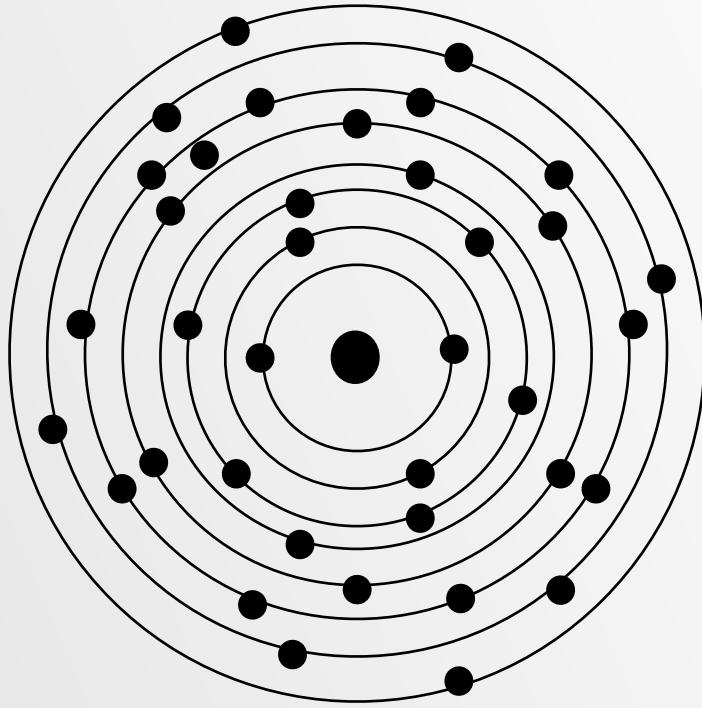
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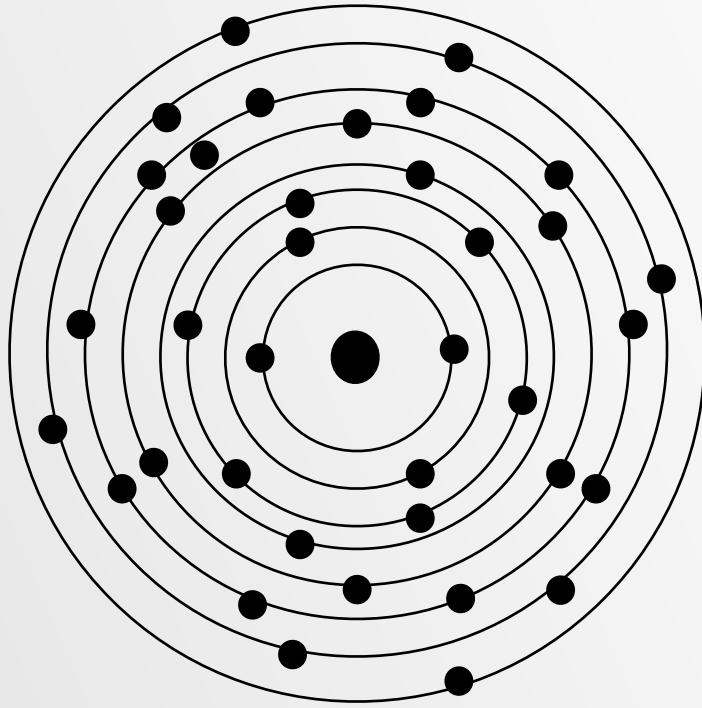
The atom as a laboratory for new physics searches



- Electromagnetic interaction
- Weak interaction
- Strong interaction

are present in atoms and may be probed and tested

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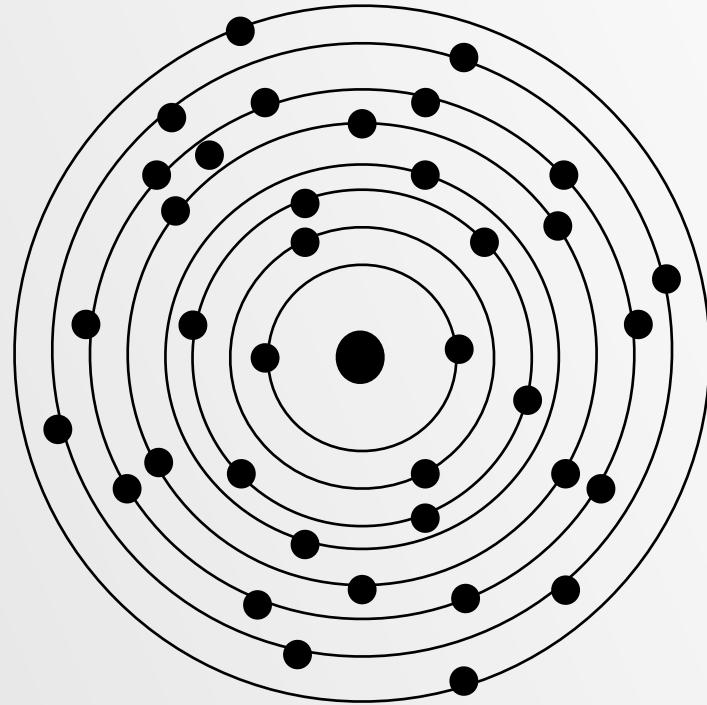
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Weak interaction does not conserve parity, $r \rightarrow -r$

May be *isolated* by studying parity-violating effects



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Complexity/simplicity of system may be varied by changing nuclear charge (Z), isotope, ionisation degree, state

- Possibilities for enhancement
- May choose more theoretically tractable system

Neutral weak currents

- Discovered at CERN (1973) in neutrino-nucleon and antineutrino-electron scattering experiments



Hadronic neutral current event: neutrino-nucleon scattering



Leptonic neutral current event: antineutrino-electron scattering

<https://cerncourier.com/a/neutral-currents-a-perfect-experimental-discovery/>

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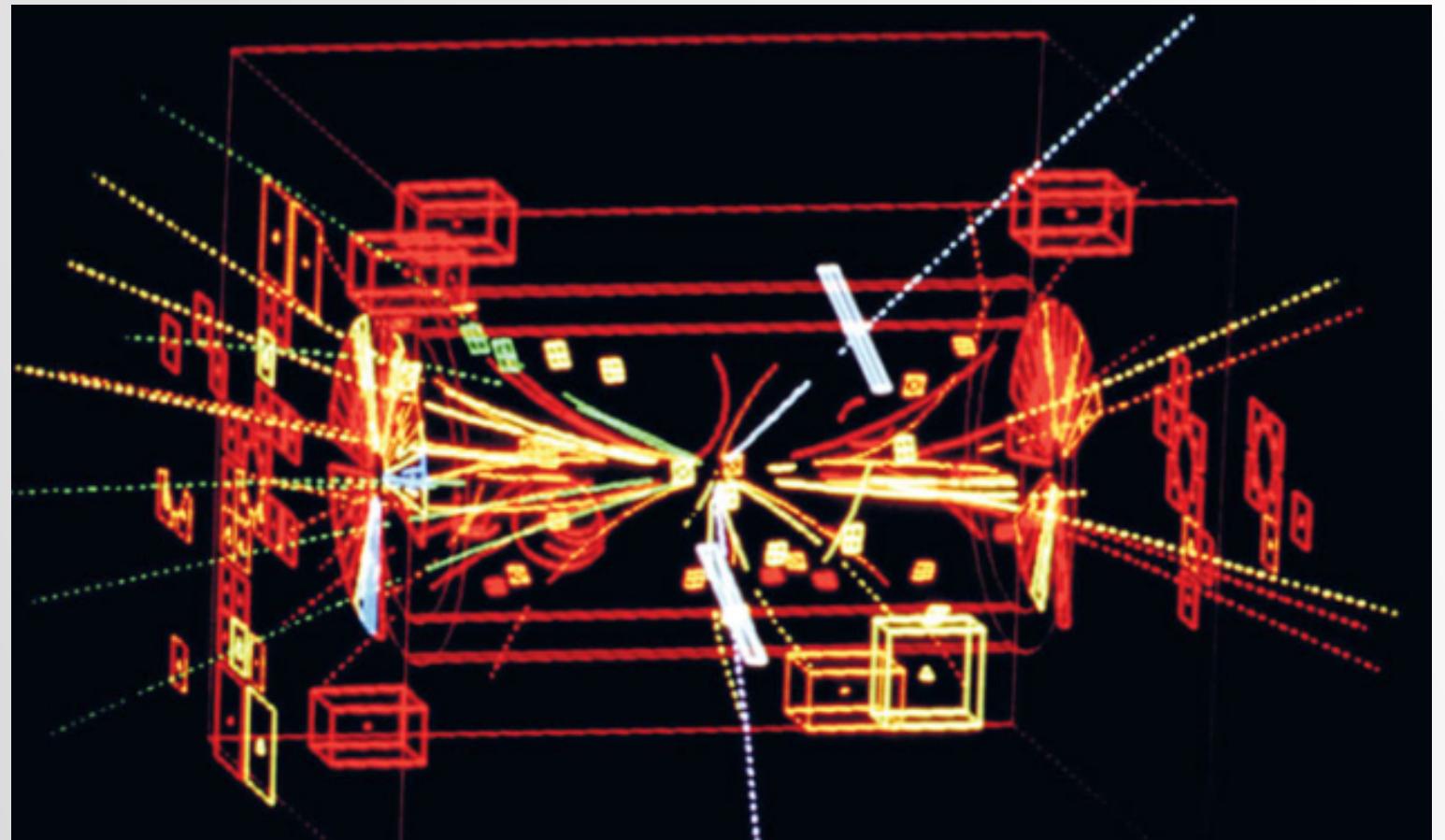


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- Z, W⁺, W⁻ produced directly at CERN (1983)

[https://cerncourier.com/
a/finding-the-w-and-z/](https://cerncourier.com/a/finding-the-w-and-z/)



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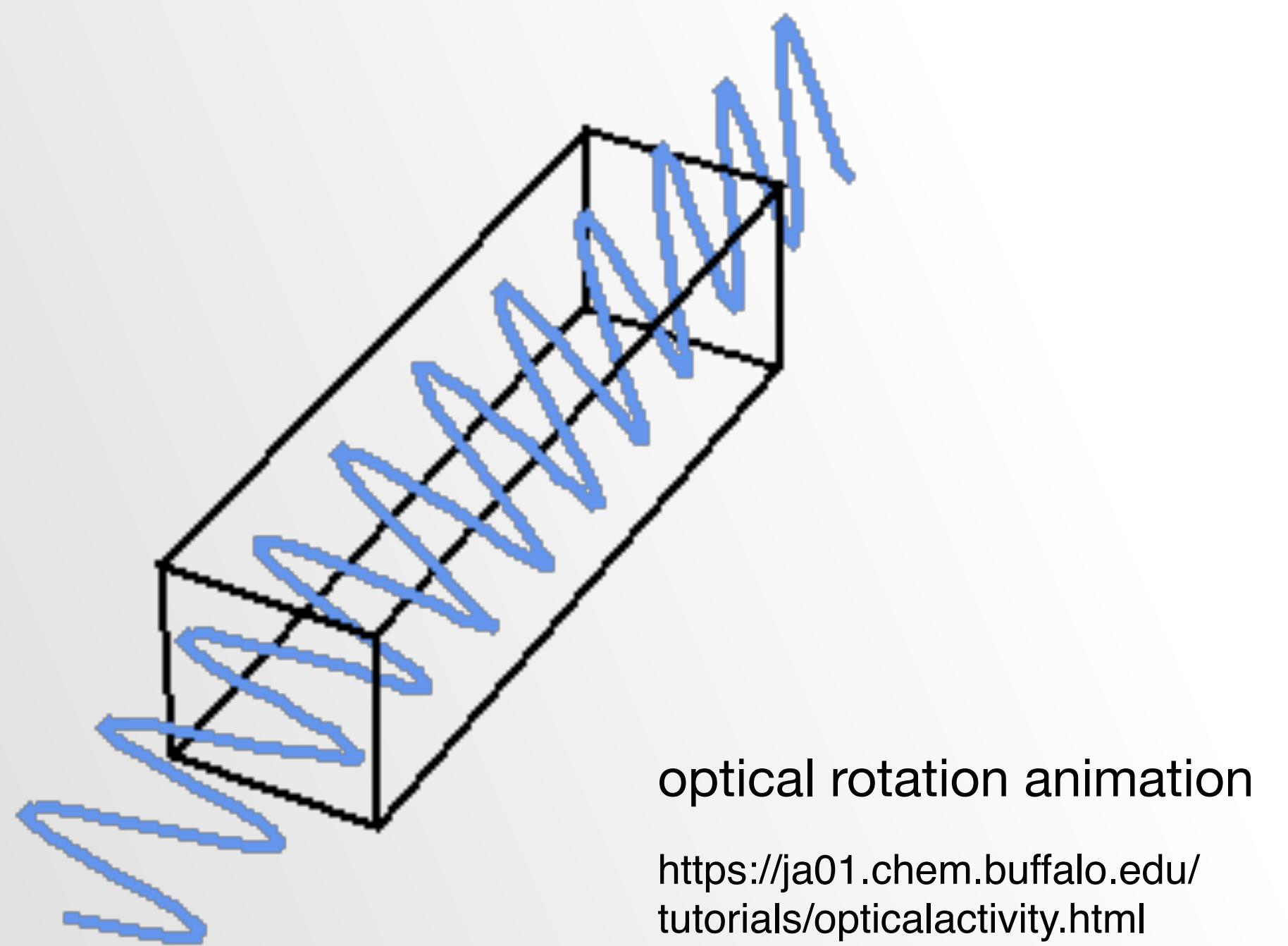


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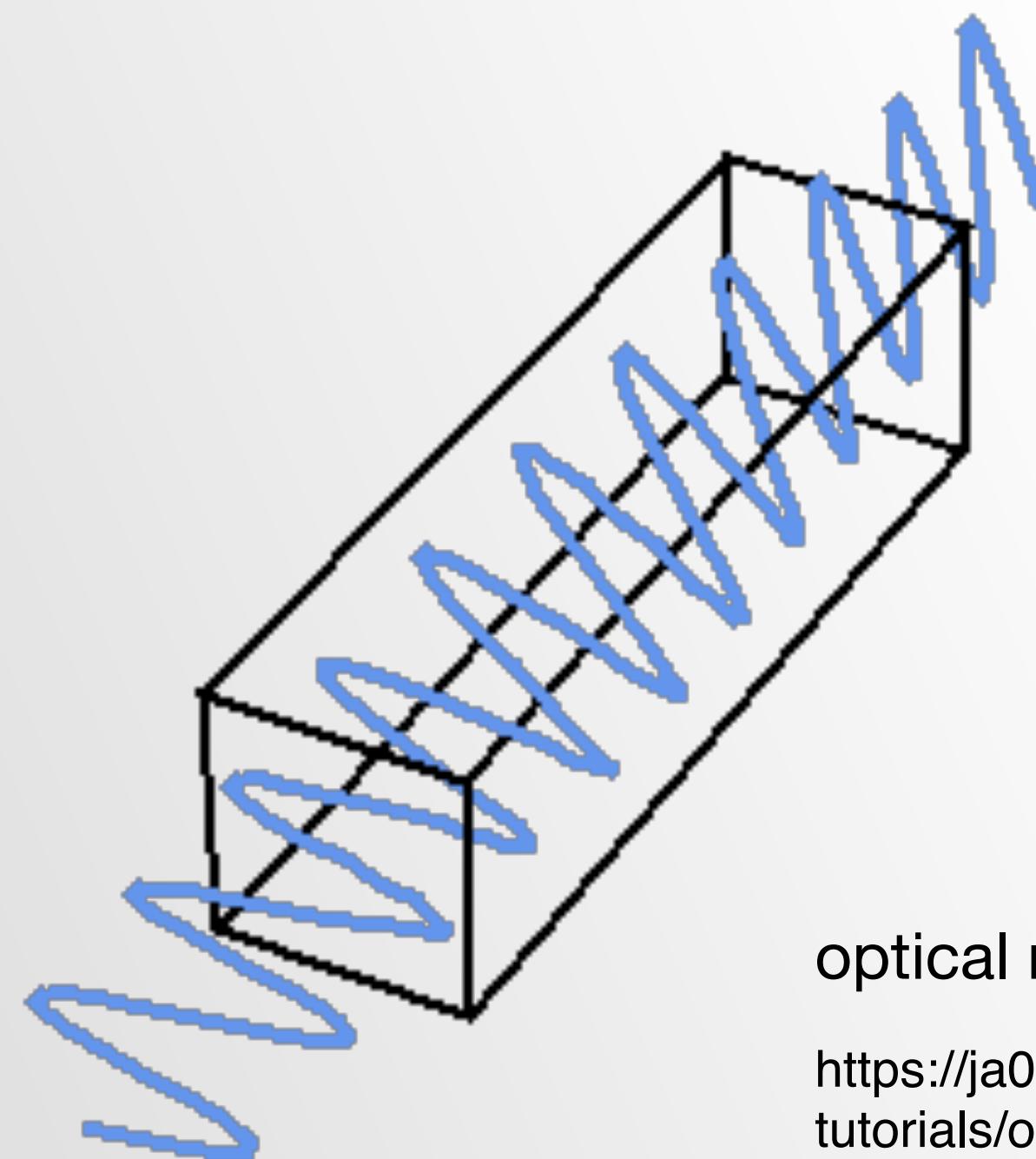
Bismuth experiment

- e-N weak interaction produces optical activity
- Plane of polarisation of light is *rotated* on passing through bismuth vapour
- *Coherent, macroscopic parity-violating effect*



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optical rotation animation

[https://ja01.chem.buffalo.edu/
tutorials/opticalactivity.html](https://ja01.chem.buffalo.edu/tutorials/opticalactivity.html)

The discovery of a new kind of a parity nonconserving weak interaction of electrons with nucleons is an example of a situation when a branch of physics (in this case, atomic spectroscopy) long since believed to be classical, again proves to be at the forefront of our understanding of nature...

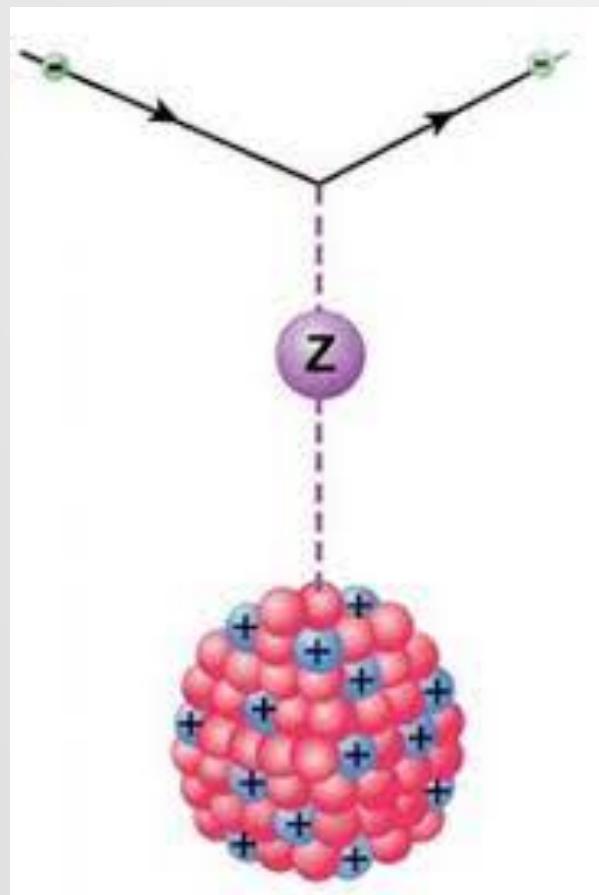
Table-top apparatus has proved to be an important addition to the experimental methods traditional for elementary particle physics. I am convinced that this case is not the last and that the time of table-top experiments in studying fundamental properties of matter is far from over.

— I. B. Khriplovich

Violations of fundamental symmetries in atoms

Precision atomic theory *needed* to extract fundamental parameters from atomic experiments for comparison with SM

Atomic parity violation (APV)



APV amplitude:

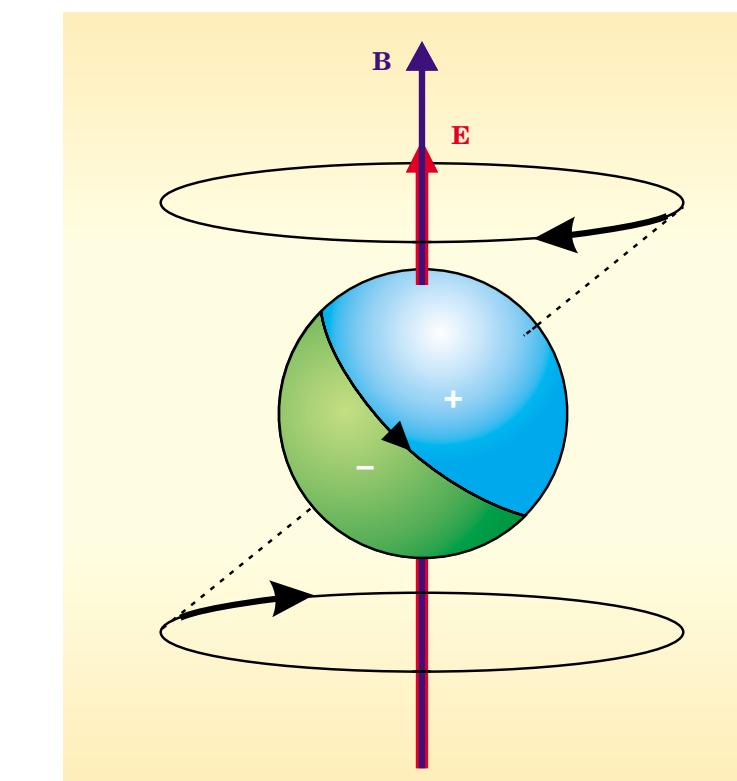
$$E_{PV} = \xi Q_w$$

from atomic
structure theory

nuclear weak
charge

Electric dipole moments (EDMs)

Parity- and time-reversal-violating



Atomic EDM:

$$d_{\text{atom}} = \zeta S + K d_e + \dots$$

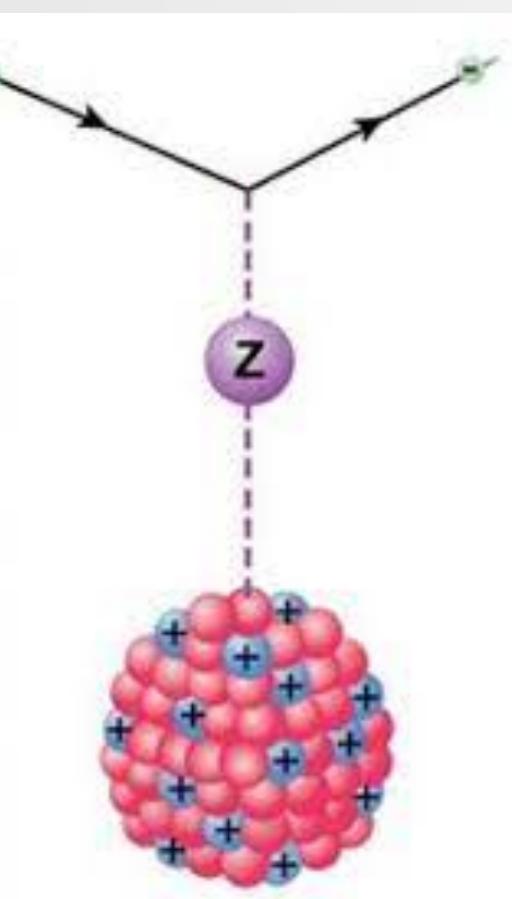
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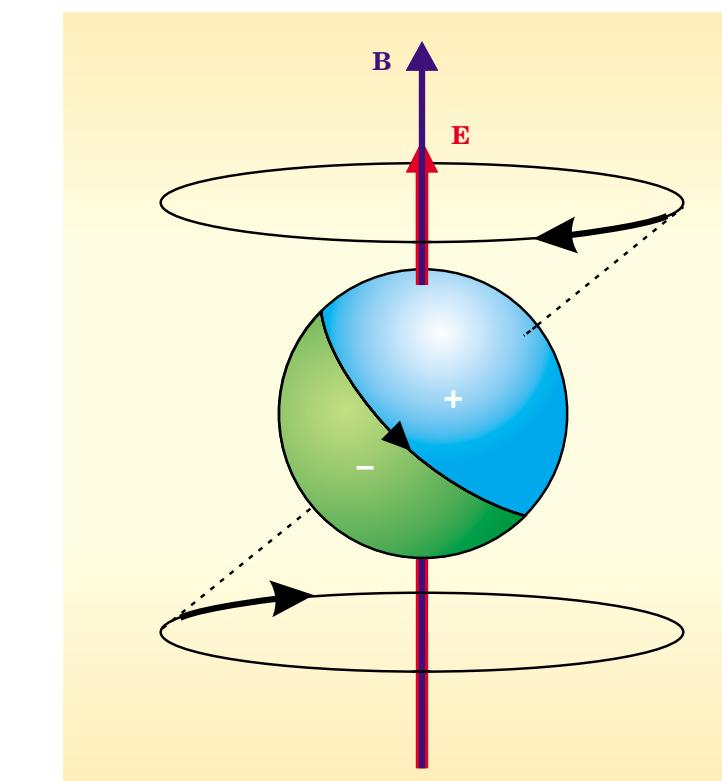
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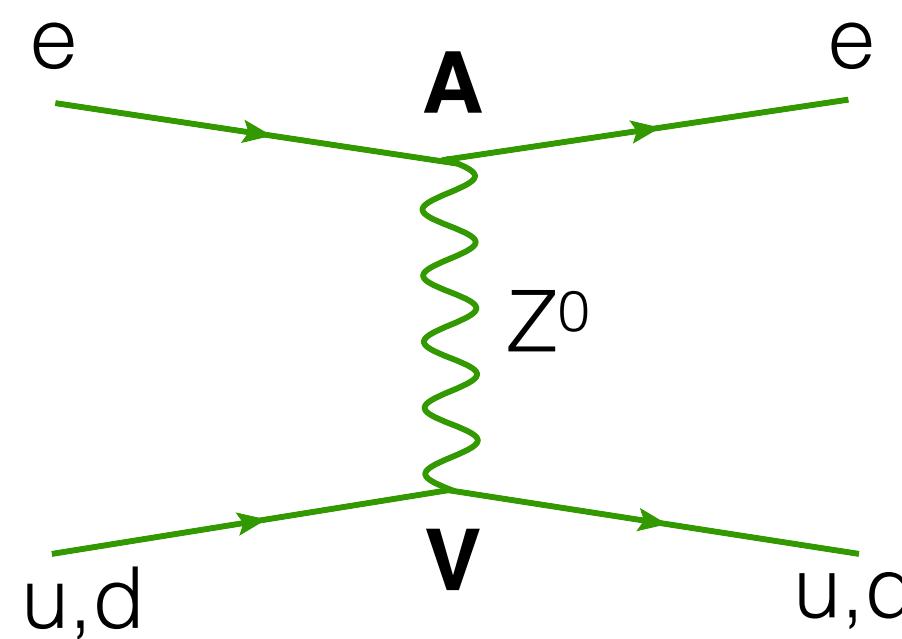
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Atomic parity violation and the nuclear weak charge

Axial vector coupling to electrons,
vector coupling to quarks

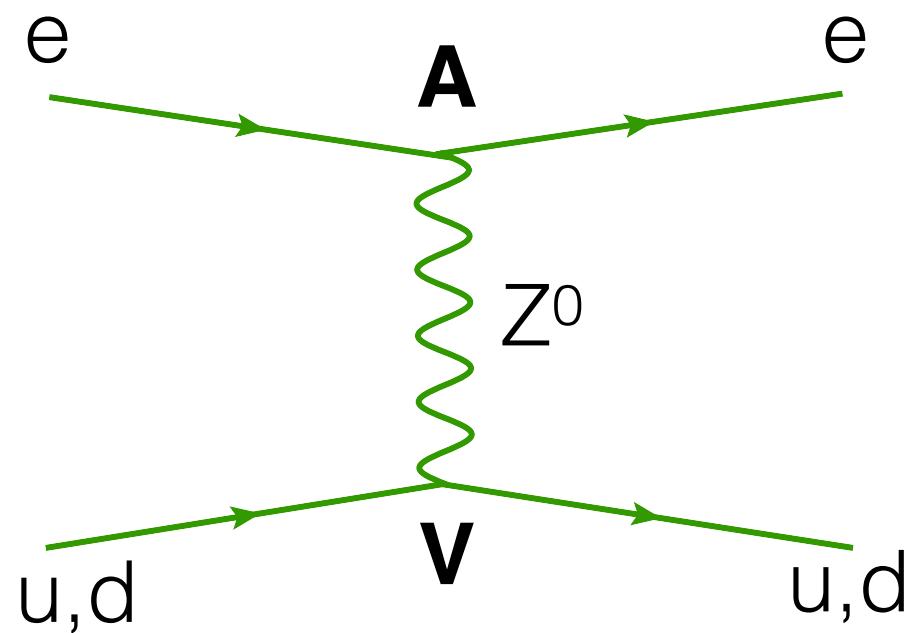
$$\frac{G}{\sqrt{2}} C_{1q} (\bar{e} \gamma_\mu \gamma_5 e) (\bar{q} \gamma^\mu q)$$



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Standard model tree-level couplings

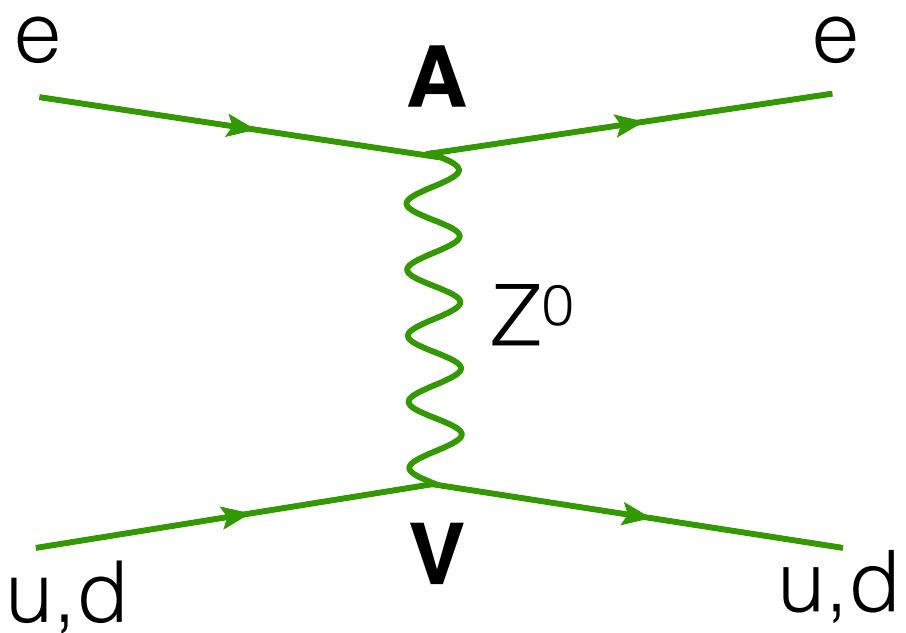
$$C_{1n} = C_{1u} + 2C_{1d} = -\frac{1}{2}$$

$$C_{1p} = 2C_{1u} + C_{1d} = \frac{1}{2}(1 - 4 \sin^2 \theta_W)$$

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Leads to parity-violating interaction Hamiltonian for electrons

$$h_{\text{PV}} = -\frac{G}{2\sqrt{2}} Q_W \rho(r) \gamma_5$$

where Q_W is *nuclear weak charge*.

SM value known well, $Q_W^{\text{SM}} = -73.23(1)$

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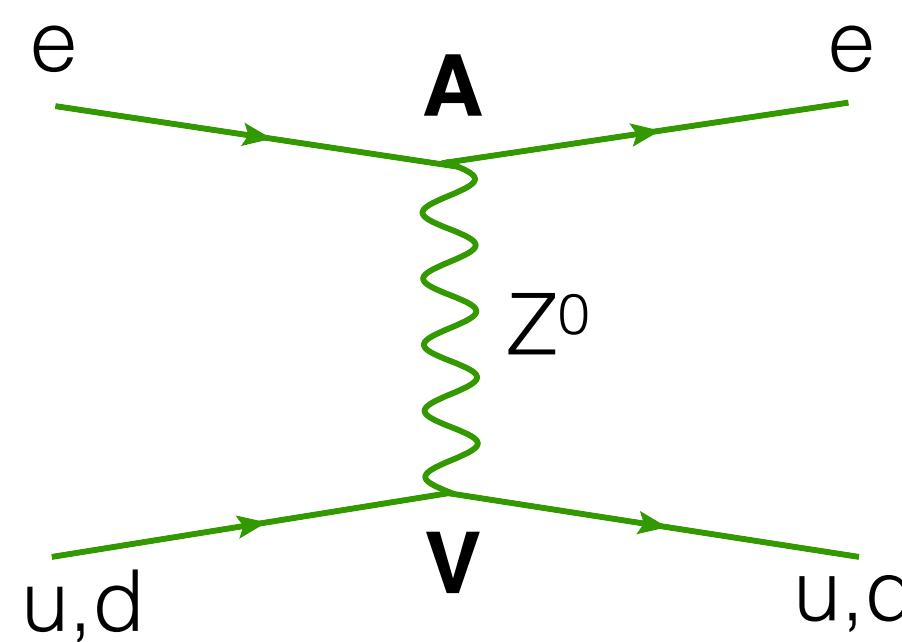
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Parity-violating nature

Non-relativistic limit:

$$h_{\text{PV}} \propto \boldsymbol{\sigma} \cdot \mathbf{p}$$

Parity operation:

$$\boldsymbol{\sigma} \rightarrow \boldsymbol{\sigma}$$

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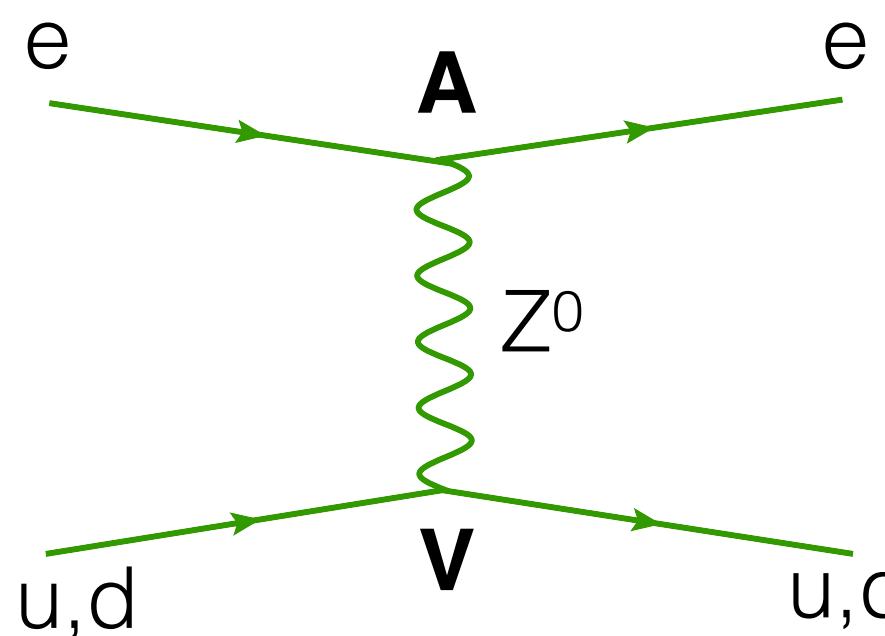
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Enhancement with Z

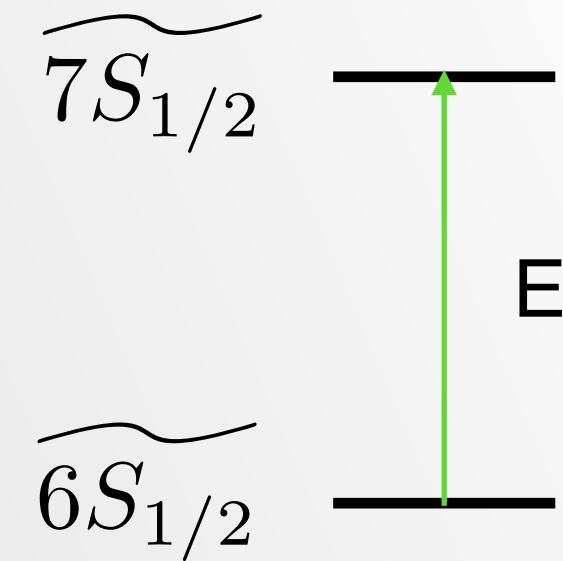
Parity-violating amplitude:

$$E_{\text{PV}} \propto R(Z) Z^3$$

relativistic
enhancement
factor

nuclear charge

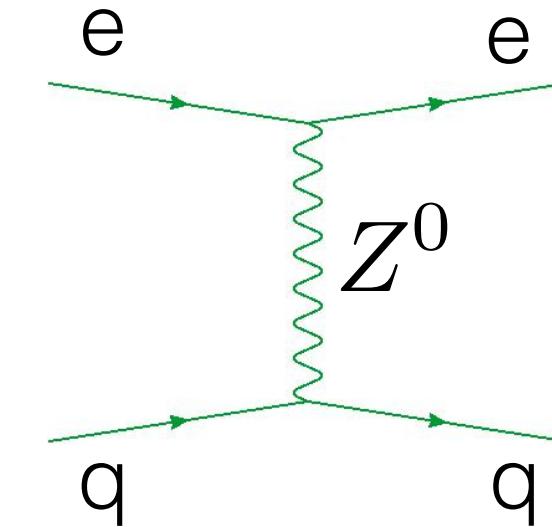
Atomic parity violation in cesium



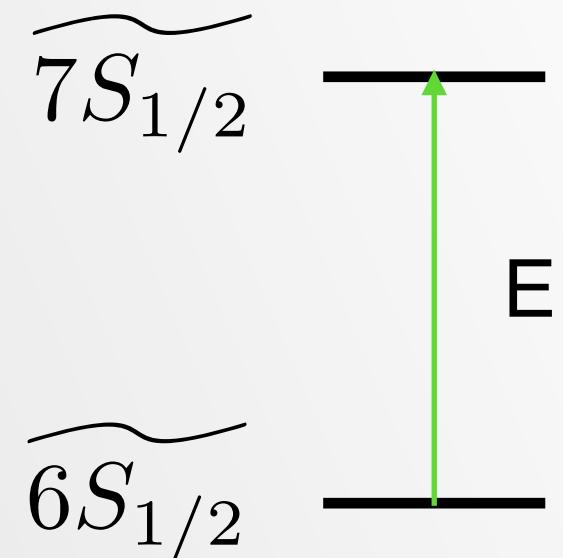
Weak interaction mixes opposite-parity states,

$$|\widetilde{S_{1/2}}\rangle = |S_{1/2}\rangle + \sum_n \frac{\langle nP_{1/2} | H_{PV} | S_{1/2} \rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} |nP_{1/2}\rangle$$

6S - 7S electric dipole (E1) transition amplitude E_{PV}



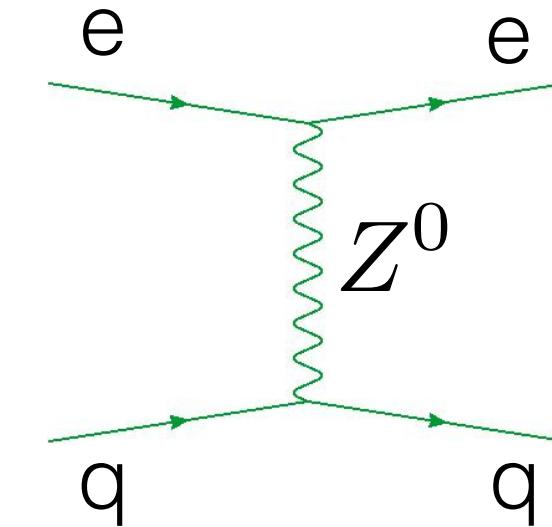
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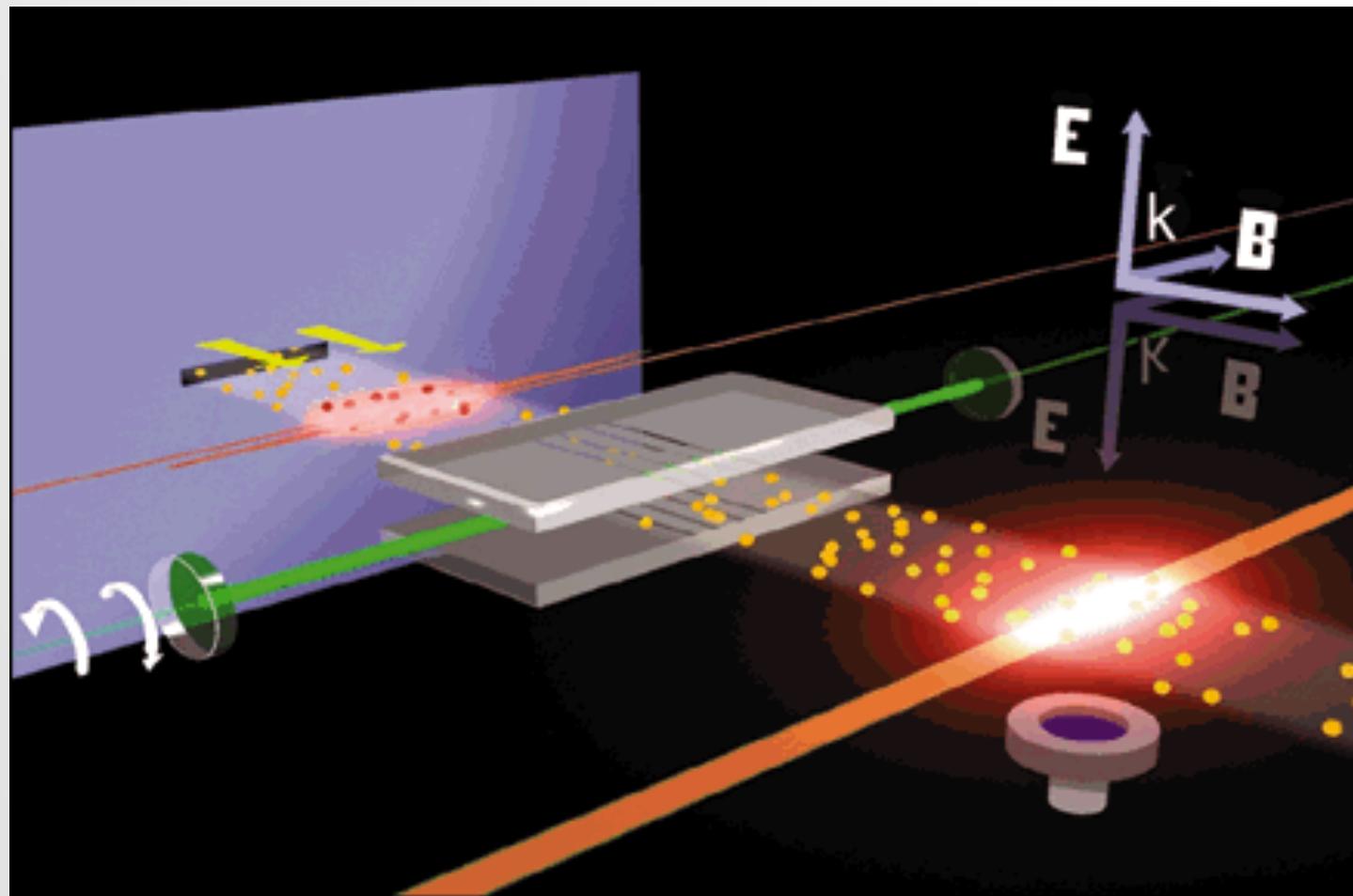
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Experiment, 0.35% uncertainty

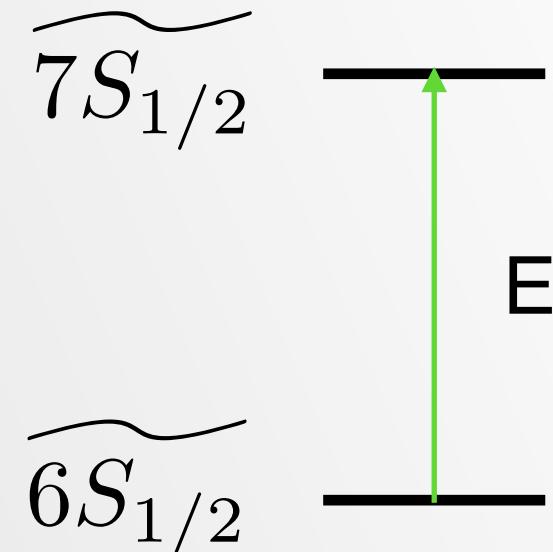


$$-\text{Im}(E_{PV})/\beta = 1.5935(1 \pm 0.35\%) \text{ mV/cm}$$

β — transition polarisability

Carl Wieman group, Wood et al., Science (1997)

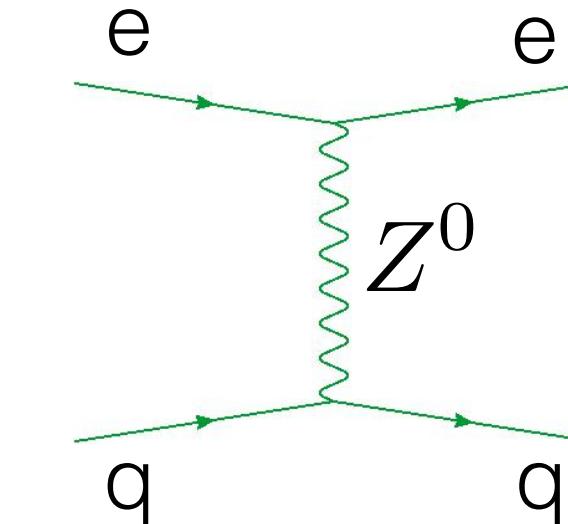
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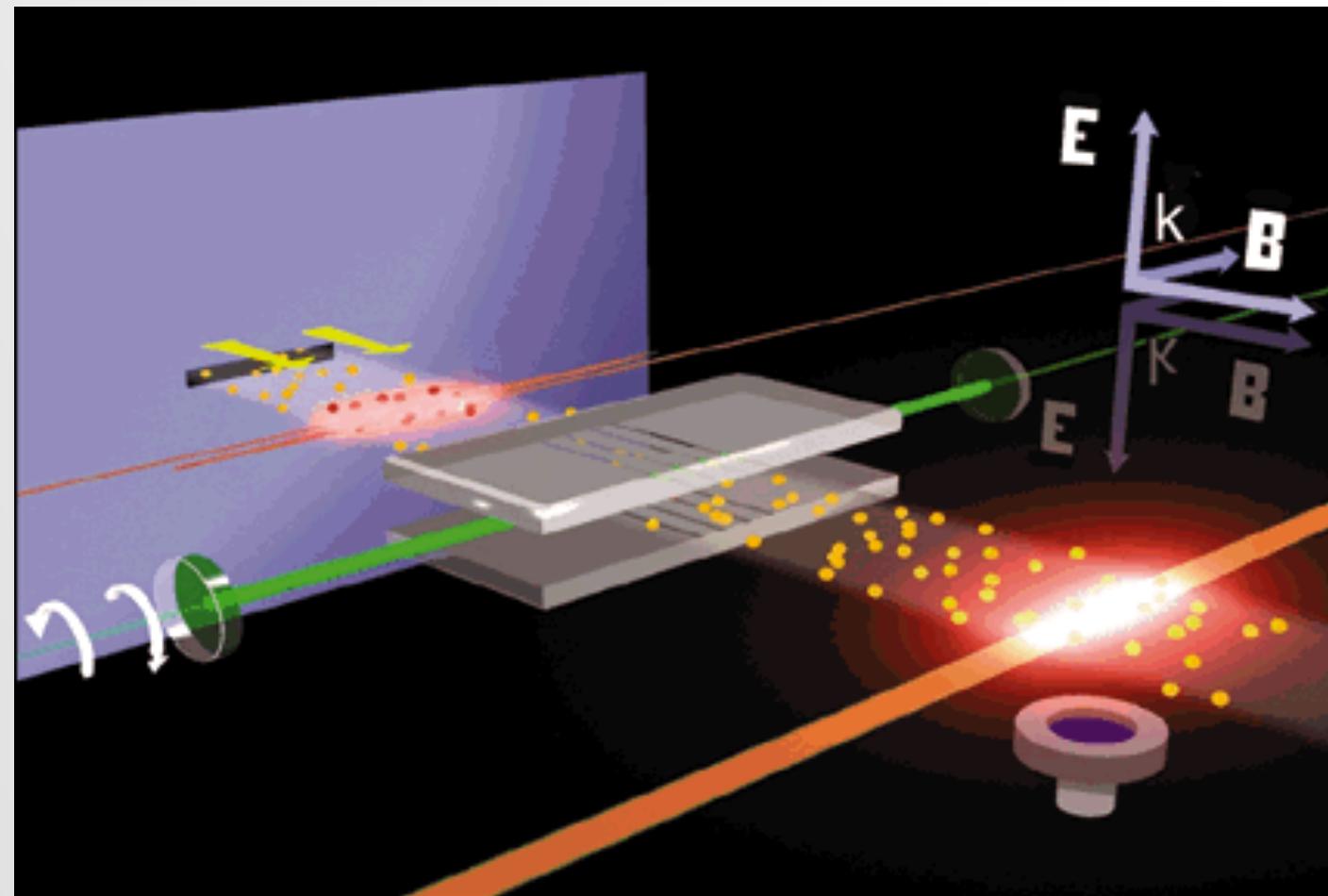
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Atomic theory, 0.5% uncertainty

$$\begin{aligned} E_{PV} &= \langle \widetilde{7S_{1/2}} | D_z | \widetilde{6S_{1/2}} \rangle \\ &= \sum_n \frac{\langle 7S_{1/2} | D_z | nP_{1/2} \rangle \langle nP_{1/2} | H_{PV} | 6S_{1/2} \rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \dots \\ &= \xi Q_W \end{aligned}$$

Dipole operator

$$\mathbf{D} = \sum_i e \mathbf{r}_i , \quad H_{PV} = \sum_i (h_{PV})_i , \quad E$$

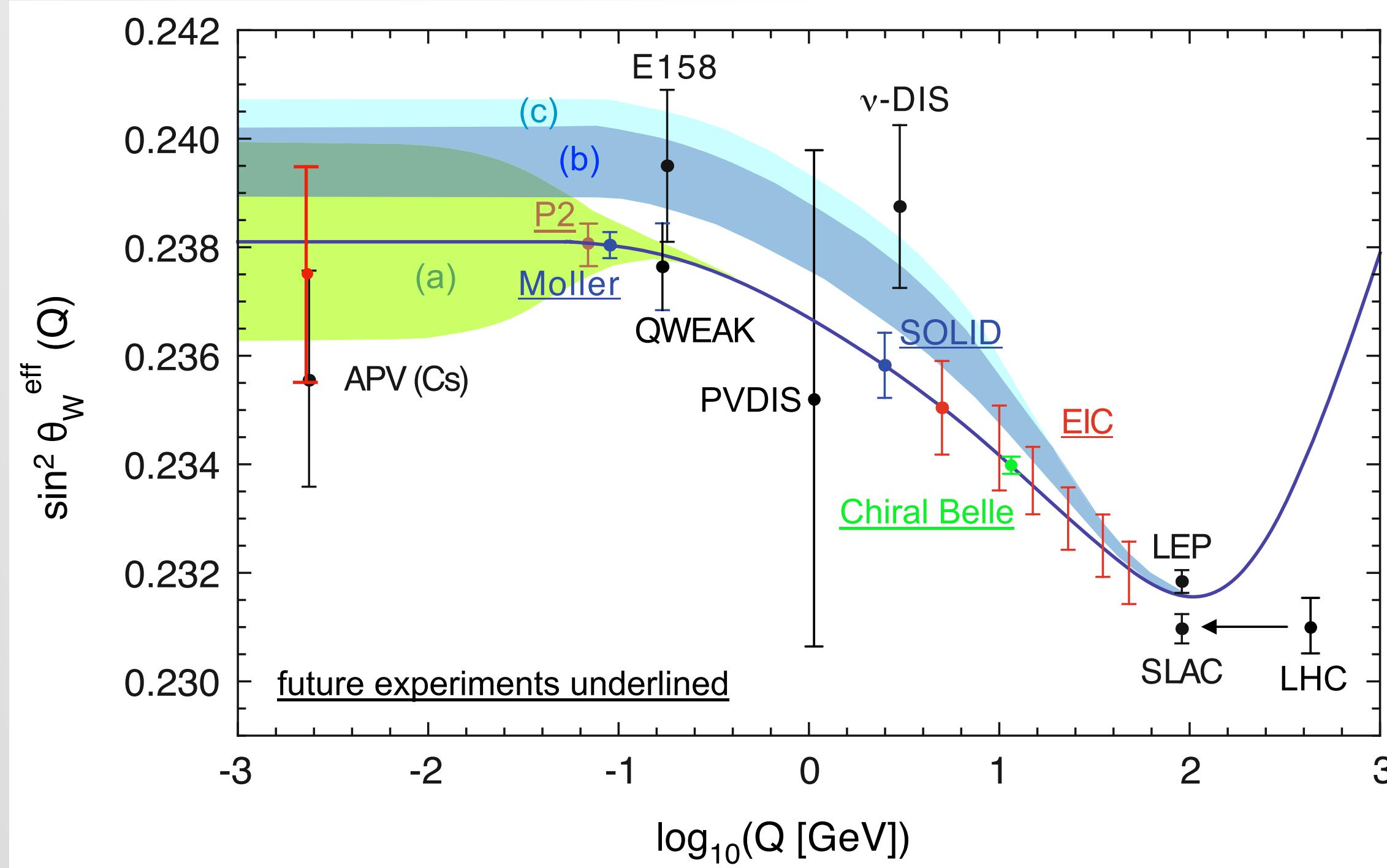
Weak operator

Dzuba, Flambaum, Ginges, PRD (2002); Flambaum, Ginges, PRA (2005)
Porsev, Beloy, Derevianko, PRL (2009); Dzuba, Berengut, Flambaum, Roberts, PRL (2012)

Tests of the standard model

- Experiment and theory: nuclear weak charge: $Q_W = -73.07(28)(33) \Rightarrow Q_W - Q_W^{\text{SM}} = 0.16(43)$

Running of the Weinberg angle



| | |
|------------|--|
| QWEAK | - electron-proton scattering |
| E158 | - electron-electron scattering @ SLAC |
| PVDIS | - parity-violation in deep inelastic scattering |
| ν -DIS | - neutrino deep inelastic scattering |
| Tevatron | - proton-antiproton collider |
| LEP | - Large Electron Positron collider |
| SLAC | - Stanford Linear Collider, electron-positron collider |
| LHC | - Large Hadron Collider, proton-proton collider |

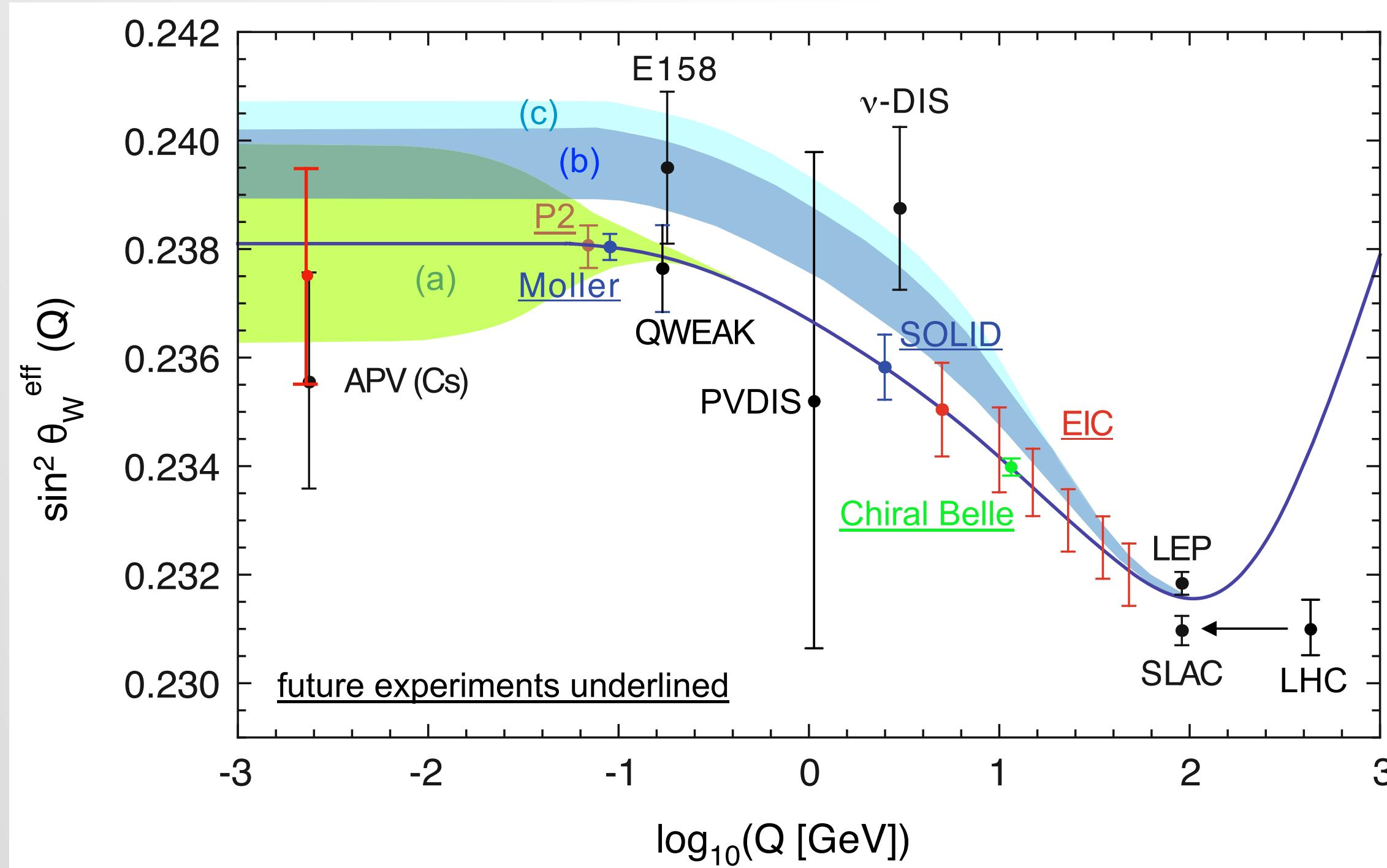
Figure from: Gwinner and Orozco, Quantum Sci. Technol (2022)

New result for vector polarizability shifts APV result (red): G. Toh et al., PRL (2019)

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Dark Z boson:
 (a) 50 MeV; (b) 15 MeV; (c) 15 MeV, in tension with expt.

Figure from: Gwinner and Orozco, Quantum Sci. Technol (2022)

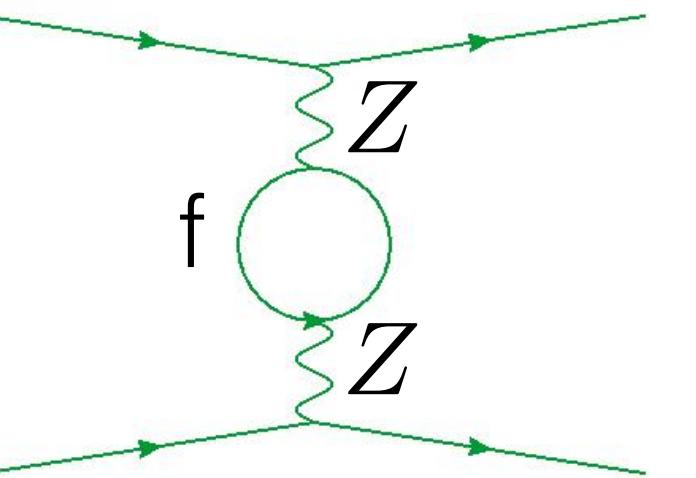
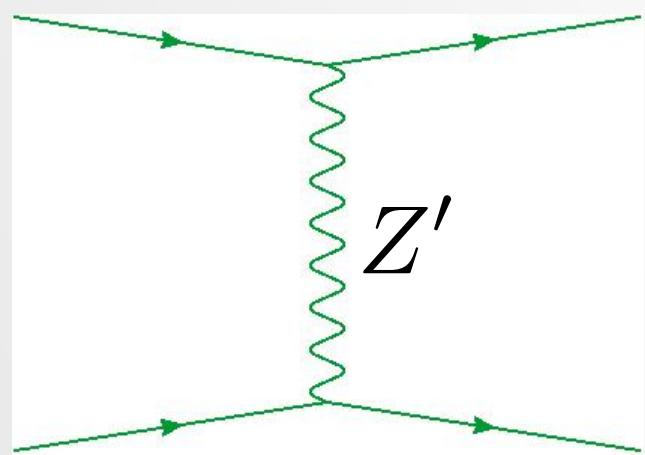
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Searches for new physics

New physics

$$Q_W = Q_W^{\text{SM}} + \Delta Q_W$$

e.g.

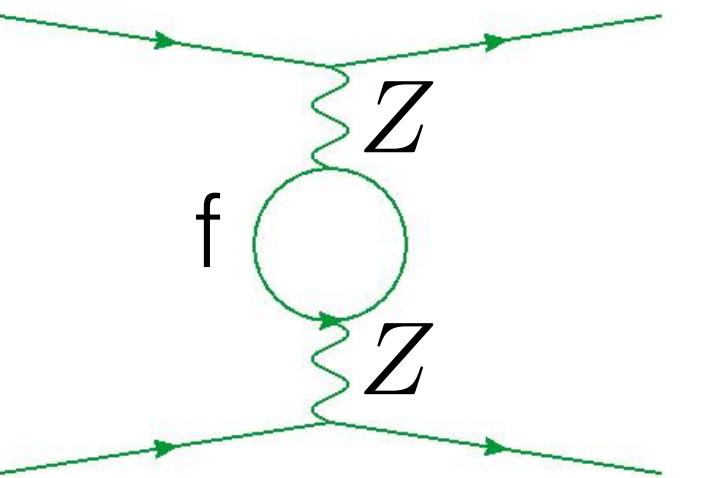
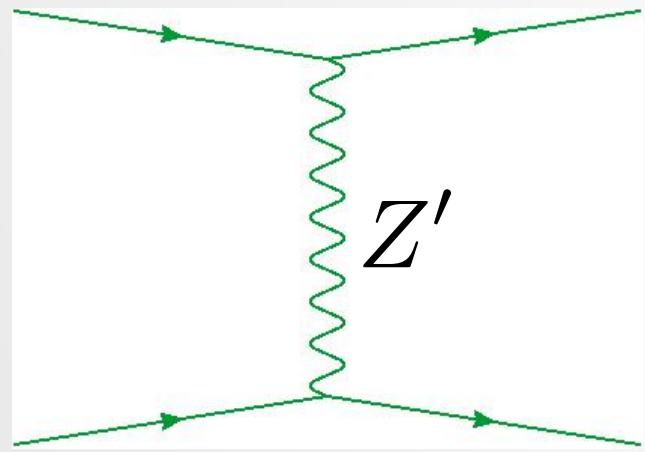


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New tree-level physics. Probing mass scale:

$$\Lambda \geq \left(\frac{8\sqrt{2}\pi\kappa^2}{(\Delta Q_W/Q_W^{\text{SM}}) G_F} \right)^{1/2}$$

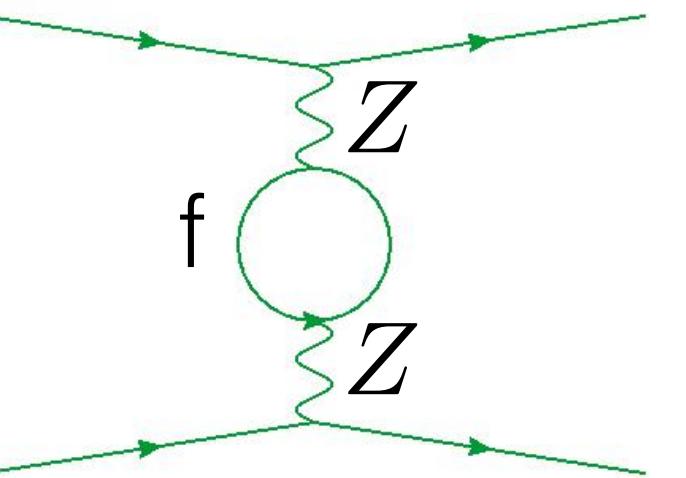
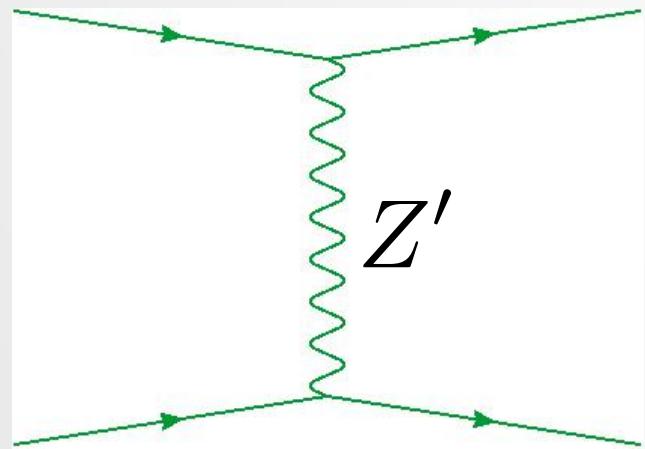
strongly interacting $\kappa^2 \sim 1$, weakly interacting $\kappa^2 \sim \alpha$

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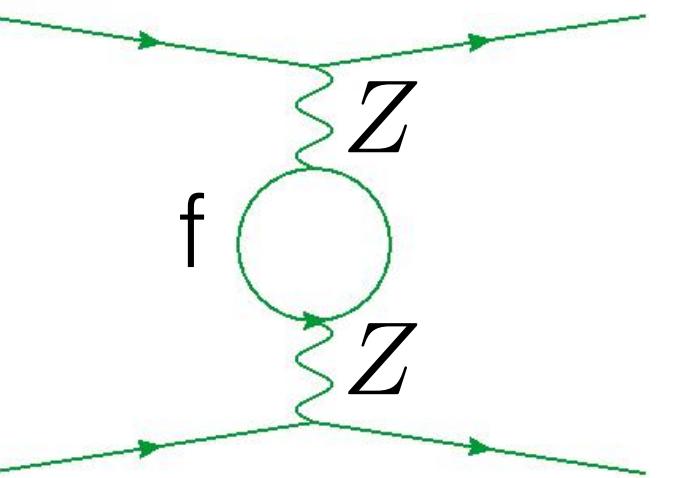
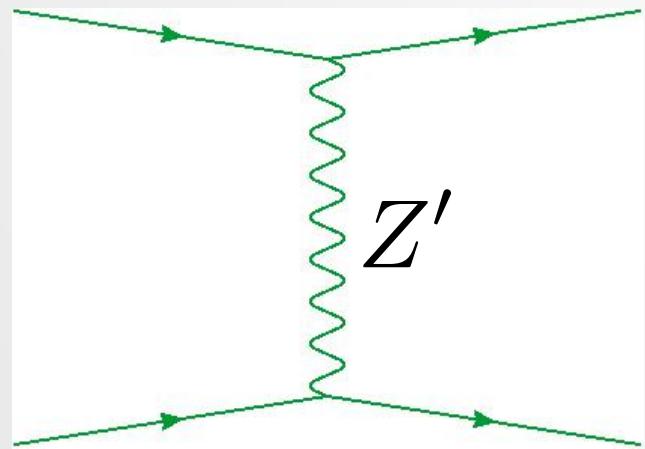
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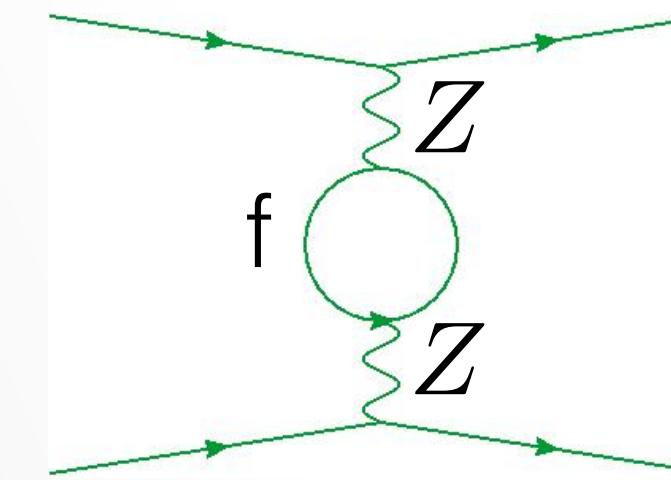
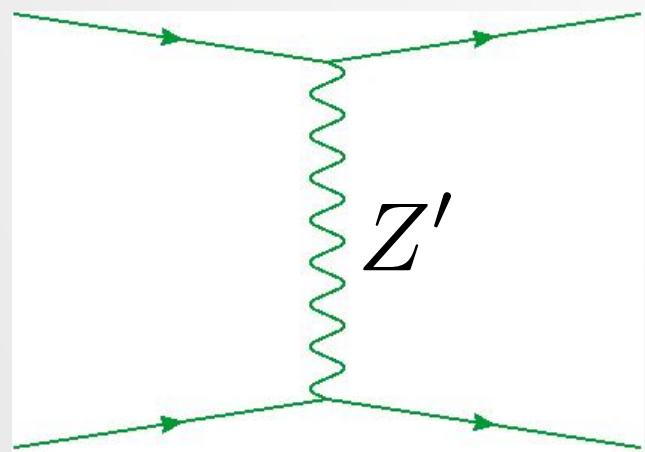
Z' boson: $m_{Z'} \gtrsim 1 \text{ TeV}$

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Ramsey-Musolf, PRC (1999)

Experiments in preparation/progress

The Periodic Table displays atomic properties and fundamental physical constants. Key features include:

- Group 1 (IA):** Hydrogen (H), Lithium (Li), Sodium (Na), Potassium (K), Rubidium (Rb), Cesium (Cs), Francium (Fr).
- Group 2 (IIA):** Helium (He), Beryllium (Be), Magnesium (Mg), Calcium (Ca), Strontium (Sr), Barium (Ba), Rutherfordium (Rf).
- Group 18 (VIIIA):** Helium (He), Nitrogen (N), Oxygen (O), Fluorine (F), Neon (Ne), Sulfur (S), Chlorine (Cl), Argon (Ar), Krypton (Kr), Xenon (Xe), Oganesson (Og).
- Period 4:** Scandium (Sc), Titanium (Ti), Vanadium (V), Chromium (Cr), Manganese (Mn), Iron (Fe), Cobalt (Co), Nickel (Ni), Copper (Cu), Zinc (Zn), Gallium (Ga), Germanium (Ge), Arsenic (As), Selenium (Se), Bromine (Br), Krypton (Kr).
- Period 5:** Yttrium (Y), Zirconium (Zr), Niobium (Nb), Molybdenum (Mo), Technetium (Tc), Ruthenium (Ru), Rhodium (Rh), Palladium (Pd), Silver (Ag), Cadmium (Cd), Indium (In), Tin (Sn), Antimony (Sb), Tellurium (Te), Iodine (I), Xenon (Xe), Radon (Rn).
- Period 6:** Hafnium (Hf), Tantalum (Ta), Tungsten (W), Rhenium (Re), Osmium (Os), Iridium (Ir), Platinum (Pt), Gold (Au), Mercury (Hg), Thallium (Tl), Lead (Pb), Bismuth (Bi), Polonium (Po), Astatine (At), Radon (Rn).
- Period 7:** Rutherfordium (Rf), Dubnium (Db), Seaborgium (Sg), Bohrium (Bh), Hassium (Hs), Meitnerium (Mt), Darmstadtium (Ds), Roentgenium (Rg), Copernicium (Cn), Nihonium (Nh), Flerovium (Fl), Moscovium (Mc), Livermorium (Lv), Tennessine (Ts), Oganesson (Og).
- Lanthanides (Ce, La, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu):** Cerium (Ce), Lanthanum (La), Praseodymium (Pr), Neodymium (Nd), Promethium (Pm), Samarium (Sm), Europium (Eu), Gadolinium (Gd), Terbium (Tb), Dysprosium (Dy), Holmium (Ho), Erbium (Er), Thulium (Tm), Ytterbium (Yb), Lutetium (Lu).
- Actinides (Ac, Th, Pa, U, Np, Pu, Am, Cf, Es, Fm, Md, No, Lr):** Actinium (Ac), Thorium (Th), Protactinium (Pa), Uranium (U), Neptunium (Np), Plutonium (Pu), Americium (Am), Curium (Cm), Berkelium (Bk), Einsteinium (Es), Fermium (Fm), Mendelevium (Md), Nobelium (No), Lawrencium (Lr).

For the most accurate values of these and other constants, visit pmi.nist.gov/constants.

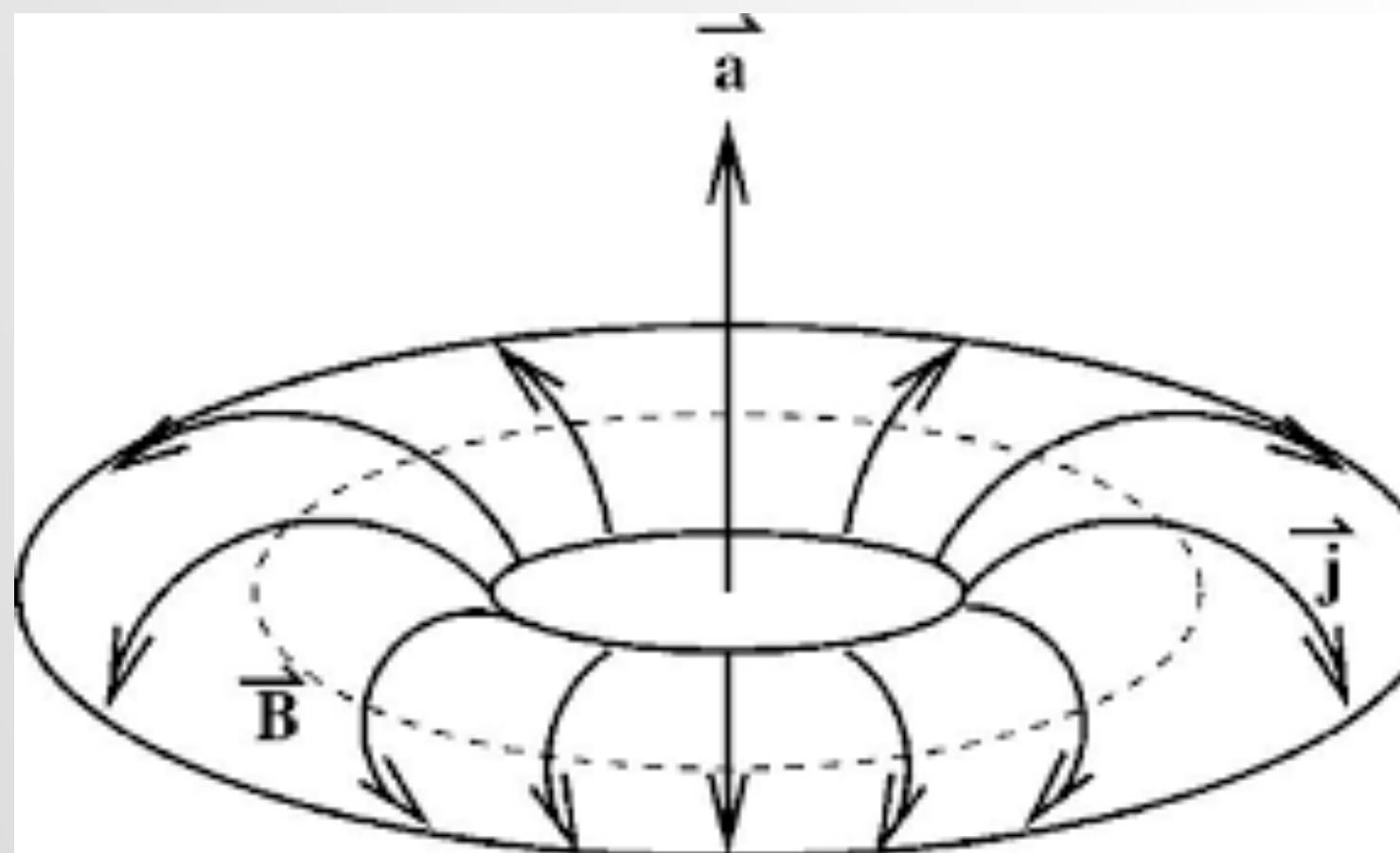
[†]Based upon ¹²C. () indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit caaw.org and pmi.nist.gov/data.

NIST SP 966 (July 2018)

Nuclear-spin-dependent

- from C_{2q} , Z-boson axial vector coupling to quarks and vector coupling to electrons:
 \Rightarrow nuclear-spin-dependent effects in atoms
- Dominated by another effect:
nuclear anapole moment, produced from parity-violating nuclear forces



Haxton and Wieman, Ann. Rev. Nuc. Part. Sci. (2001)

Flambaum and Ginges, Phys. Rep. (2004)

Experiments in preparation/progress

P E R I O D I C T A B L E
Atomic Properties of the Elements

NIST National Institute of Standards and Technology
U.S. Department of Commerce

Physical Measurement Laboratory www.nist.gov/pml
Standard Reference Data www.nist.gov/srd

18
VIIIA

| |
|--|
| 2 1s ₀ He Helium 4.0028 1s ¹ 24.5674 |
| 13 IIIA Boron 10.81 1s ² 2s ² 8.2860 |
| 14 IVA Carbon 12.011 1s ² 2s ² 2p ² 14.5941 |
| 15 VA Nitrogen 14.007 1s ² 2s ² 2p ³ 18.998 |
| 16 VIA Oxygen 15.998 1s ² 2s ² 2p ⁴ 13.0181 |
| 17 VIIA Fluorine 18.998 1s ² 2s ² 2p ⁵ 17.4228 |
| 10 1s ₀ Neon 20.180 1s ² 2s ² 2p ⁶ 21.5646 |
| 5 2p _{1/2} B 10.81 1s ² 2s ² 2p ¹ 8.2860 |
| 6 3p ₀ C 12.011 1s ² 2s ² 2p ² 14.5941 |
| 7 4s _{1/2} N 14.007 1s ² 2s ² 2p ³ 18.998 |
| 8 3p ₂ O 15.998 1s ² 2s ² 2p ⁴ 13.0181 |
| 9 2p _{3/2} F 17.4228 |
| 13 2p _{1/2} Aluminum 26.982 [Ne]3s ² 3p ¹ 10.3947 |
| 14 3p ₀ Silicon 28.085 [Ne]3s ² 3p ² 11.2003 |
| 15 4s _{1/2} Phosphorus 30.974 [Ne]3s ² 3p ³ 12.4228 |
| 16 3p ₂ Sulfur 32.08 [Ne]3s ² 3p ⁴ 13.6181 |
| 17 2p _{3/2} Chlorine 35.45 [Ne]3s ² 3p ⁵ 12.9876 |
| 18 1s ₀ Argon 39.948 [Ne]3s ² 3p ⁶ 15.7508 |
| 31 2p _{1/2} Gallium 68.723 [Ar]3d ¹⁰ 4s ² 10.3947 |
| 32 3p ₀ Germanium 72.630 [Ar]3d ¹⁰ 4s ² 11.2003 |
| 33 4s _{1/2} Arsenic 74.922 [Ar]3d ¹⁰ 4s ³ 12.4228 |
| 34 3p ₂ Selenium 78.971 [Ar]3d ¹⁰ 4s ⁴ 13.6181 |
| 35 2p _{3/2} Krypton 83.798 [Ar]3d ¹⁰ 4s ⁵ 14.8087 |
| 50 3p ₀ Bromine 79.904 [Ar]3d ¹⁰ 4s ⁶ 15.998 |
| 51 4s _{1/2} Xenon 118.71 [Ar]3d ¹⁰ 4s ⁷ 17.4228 |
| 52 3p ₂ Iodine 121.76 [Ar]3d ¹⁰ 4s ⁸ 18.998 |
| 53 2p _{3/2} Tellurium 127.80 [Ar]3d ¹⁰ 4s ⁹ 20.180 |
| 54 1s ₀ Xe 131.29 [Ar]3d ¹⁰ 4s ¹⁰ 21.5646 |
| 55 2s _{1/2} Cs 132.91 [Xe]4f ¹⁴ 5d ¹ 6s ¹ 5.2117 |
| 56 1s ₀ Barium 137.33 [Xe]4f ¹⁴ 5d ² 6.5815 |
| 72 3f ₂ Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s ² 8.2851 |
| 73 4f _{3/2} Tantalum 180.95 [Xe]4f ¹⁴ 5d ³ 6s ² 7.5496 |
| 74 5d ₀ Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s ² 7.8940 |
| 75 6s ₂ Rhenium 186.21 [Xe]4f ¹⁴ 5d ⁵ 6s ² 7.7194 |
| 76 5d ₄ Technetium 192.23 [Xe]4f ¹⁴ 5d ⁶ 6s ² 7.4832 |
| 77 6f _{5/2} Ruthenium 194.24 [Xe]4f ¹⁴ 5d ⁷ 6s ² 7.9870 |
| 78 7d ₃ Rhodium 192.91 [Xe]4f ¹⁴ 5d ⁸ 6s ² 7.5489 |
| 79 7s ₂ Rhodium 195.08 [Xe]4f ¹⁴ 5d ⁹ 6s ² 8.0688 |
| 80 8s ₀ Platinum 196.97 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 10.4375 |
| 81 2p _{1/2} Gold 199.97 [Xe]4f ¹⁴ 5d ¹⁰ 6s ³ 10.2250 |
| 82 3p ₀ Mercury 200.59 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁴ 10.4913 |
| 83 4s _{1/2} Thallium 204.38 [Hg]6p ¹ 7.2855 |
| 84 3p ₂ Lead 207.2 [Hg]6p ² 8.414 |
| 85 2p _{3/2} Bismuth 208.88 [Hg]6p ³ 9.3175 |
| 86 1s ₀ Radon (222) [Hg]6p ⁸ 10.7485 |
| 58 1g ₄ Ce 140.12 [Xe]4f ¹⁴ 5d ⁵ 6s ² 5.5386 |
| 59 4f _{9/2} Praseodymium 140.91 [Xe]4f ¹⁴ 5d ⁶ 6s ² 5.4702 |
| 60 5t ₄ Neodymium 144.24 [Xe]4f ¹⁴ 5d ⁷ 6s ² 5.5250 |
| 61 6s ₂ Promethium 145.06 [Xe]4f ¹⁴ 5d ⁸ 6s ² 5.5577 |
| 62 7f ₀ Samarium 150.36 [Xe]4f ¹⁴ 5d ⁹ 6s ² 5.6437 |
| 63 8s ₀ Europium 151.98 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 5.6704 |
| 64 9s ₂ Gadolinium 157.25 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁴ 5.6498 |
| 65 5h _{15/2} Terbium 158.93 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁵ 5.6838 |
| 66 5t ₈ Dysprosium 162.50 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁶ 6.0215 |
| 67 6s ₂ Holmium 164.93 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁷ 6.1077 |
| 68 7s ₂ Erbium 167.26 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁸ 6.1843 |
| 69 7t ₂ Thulium 168.93 [Xe]4f ¹⁴ 5d ¹⁰ 6s ⁹ 6.2542 |
| 70 1s ₀ Ytterbium 173.05 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹⁰ 6.4259 |
| 71 3d ₂ Lutetium 174.97 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹² 6.5800 |
| 91 4t _{1/2} Actinium 231.04 [Rn]5f ¹⁴ 6d ⁷ s ² 5.89 |
| 92 5l _{-1/2} Thorium 232.04 [Rn]5f ¹⁴ 6d ⁷ s ² 6.0191 |
| 93 6l _{-1/2} Protactinium 234.03 [Rn]5f ¹⁴ 6d ⁷ s ² 6.2665 |
| 94 7f ₀ Uranium 237 [Rn]5f ¹⁴ 6d ⁷ s ² 5.9738 |
| 95 8s ₀ Plutonium 244 [Rn]5f ¹⁴ 6d ⁷ s ² 6.0258 |
| 96 9s ₂ Curium 247 [Rn]5f ¹⁴ 6d ⁷ s ² 5.9914 |
| 97 6h _{15/2} Berkelium 247 [Rn]5f ¹⁴ 6d ⁷ s ² 6.1978 |
| 98 7t ₈ Einsteinium 252 [Rn]5f ¹⁴ 6d ⁷ s ² 6.2817 |
| 99 8t _{1/2} Fermium 257 [Rn]5f ¹⁴ 6d ⁷ s ² 6.50 |
| 100 3h ₆ Mendelevium 262 [Rn]5f ¹⁴ 6d ⁷ s ² 6.58 |
| 101 2t _{7/2} Nobelium 268 [Rn]5f ¹⁴ 6d ⁷ s ² 4.96 |
| 102 1s ₀ Lawrencium (260) [Rn]5f ¹⁴ 6d ⁷ s ² 6.66 |
| 103 2p _{1/2} Lanthanides [Rn]5f ¹⁴ 5d ¹ 6s ² 5.5393 |
| 104 3f _{7/2} Actinides [Rn]5f ¹⁴ 5d ² 6s ² 6.02 |

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS[§]

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs (exact)

c speed of light in vacuum
h Planck constant
e elementary charge
m_e electron mass
m_ec² 0.510 998 MeV
m_p proton mass
α fine-structure constant
Rydberg constant
R_∞ c²/hc
R_∞ hc 13.605 693 eV
electron volt
Boltzmann constant
molar gas constant

For the most accurate values of these and other constants, visit physics.nist.gov/cuu/Constants/

Solids
Liquids
Gases
Artificially Prepared

[§]Based upon ¹²C. () indicates the mass number of the longest-lived isotope.

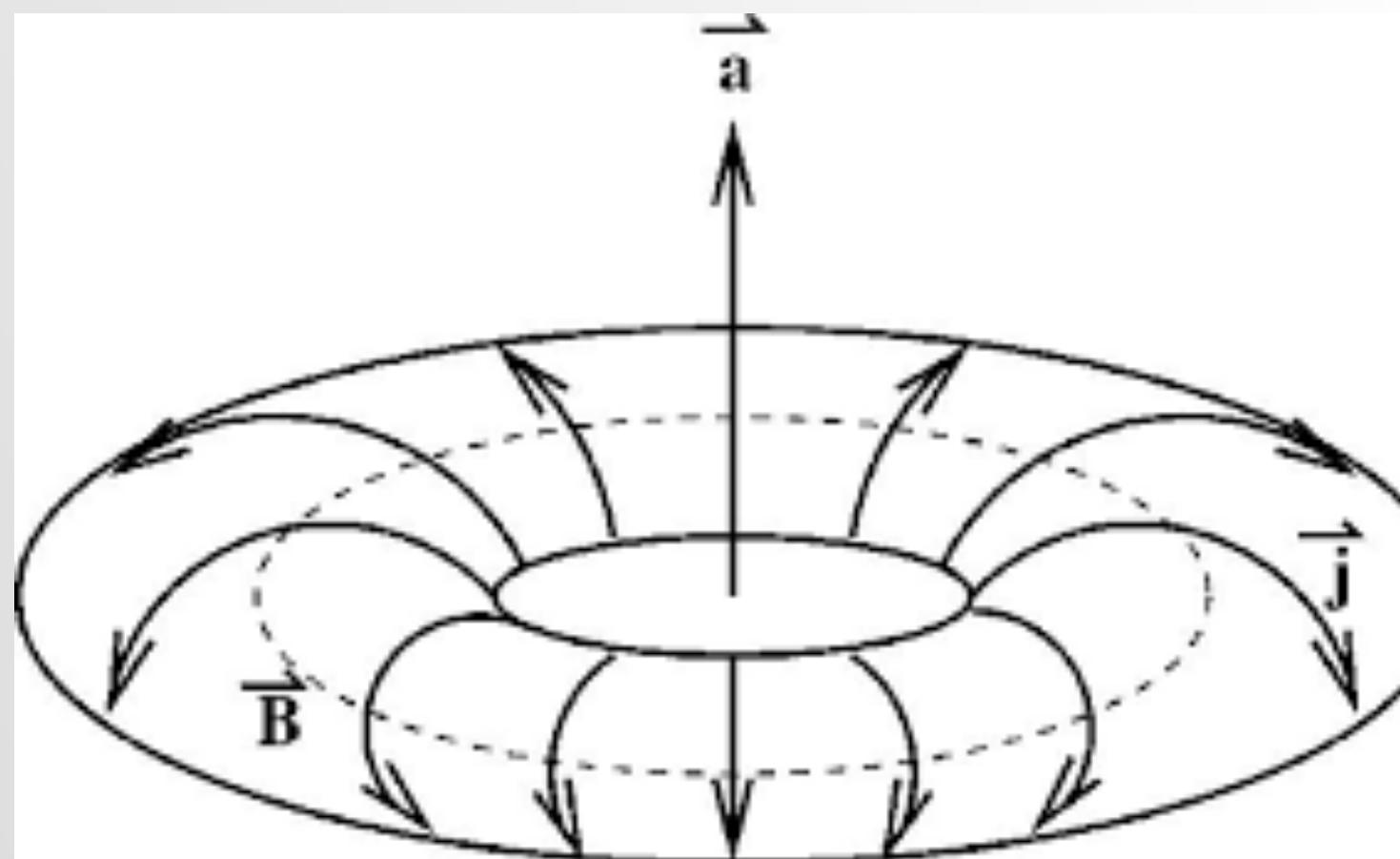
For the most precise values and uncertainties visit casaaw.org and pmi.nist.gov/data/.

NIST SP 966 (July 2018)

Neutral atoms: Cs (Purdue) ; Fr (TRIUMF; Tokyo)
Singly-ionized atoms: Ba⁺ (Seattle) ; Ra⁺ (Groningen)

Nuclear-spin-dependent

- from C_{2q} , Z-boson axial vector coupling to quarks and vector coupling to electrons:
 \Rightarrow *nuclear-spin-dependent* effects in atoms
 - Dominated by another effect:
nuclear anapole moment, produced from parity-violating nuclear forces



Experiments in preparation/progress

The Periodic Table displays the following information:

- Group 1 (IA):** Hydrogen (H) and Helium (He).
- Group 2 (IIA):** Lithium (Li), Beryllium (Be), Boron (B), Carbon (C), Nitrogen (N), Oxygen (O), Fluorine (F), and Neon (Ne).
- Group 3 (IIIB):** Sodium (Na), Magnesium (Mg), Scandium (Sc), Titanium (Ti), Vanadium (V), Chromium (Cr), Manganese (Mn), Iron (Fe), Cobalt (Co), Nickel (Ni), Copper (Cu), Zinc (Zn), Gallium (Ga), Germanium (Ge), Arsenic (As), Selenium (Se), Bromine (Br), and Krypton (Kr).
- Group 4 (IVB):** Potassium (K), Calcium (Ca), Rubidium (Rb), Strontium (Sr), Yttrium (Y), Zirconium (Zr), Niobium (Nb), Molybdenum (Mo), Technetium (Tc), Ruthenium (Ru), Rhodium (Rh), Palladium (Pd), Silver (Ag), Cadmium (Cd), Indium (In), Tin (Sn), Antimony (Sb), Tellurium (Te), Iodine (I), Xenon (Xe), and Radon (Rn).
- Group 5 (VIB):** Francium (Fr), Radium (Ra), Rutherfordium (Rf), Dubnium (Db), Seaborgium (Sg), Bohrium (Bh), Hassium (Hs), Meitnerium (Mt), Darmstadtium (Ds), Roentgenium (Rg), Copernicium (Cn), Nihonium (Nh), Flerovium (Fl), Moscovium (Mc), Livermorium (Lv), Tennessine (Ts), and Oganesson (Og).
- Group 6 (VIIB):** Lanthanides (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) and Actinides (Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr).
- Physical Constants:** Speed of light in vacuum, Planck constant, elementary charge, electron mass, proton mass, fine-structure constant, Rydberg constant, electron volt, Boltzmann constant, molar gas constant.
- Legend:** Solids (white), Liquids (purple), Gases (red), Artificially Prepared (blue).
- NIST Logo:** National Institute of Standards and Technology, U.S. Department of Commerce.
- Physical Measurement Laboratory:** www.nist.gov/pml
- Standard Reference Data:** www.nist.gov/srd

Also APV along an isotope chain! Remove dependence on atomic theory

Haxton and Wieman, Ann. Rev. Nucl. Part. Sci. (2001)

Flambaum and Ginges, Phys. Rep. (2004)

Budker group, Mainz: Yb, Dy. D. Antypas et al., Nature Physics (2019)

FrPNC collaboration: Fr

Overview

Testing the SM and searching for new physics in atoms

- Atomic parity violation
- Time-reversal-violating electric dipole moments

Adventures at the intersection of atomic and nuclear physics

- Case study in the hyperfine structure



Our precision atomic theory group at UQ – goal

To maximise the discovery potential of precision atomic experiments

- Push state-of-the-art atomic calculations to 0.1% precision
 - Development of high-precision many-body methods
 - Improved benchmarking of atomic theory

Our precision atomic theory group at UQ – goal

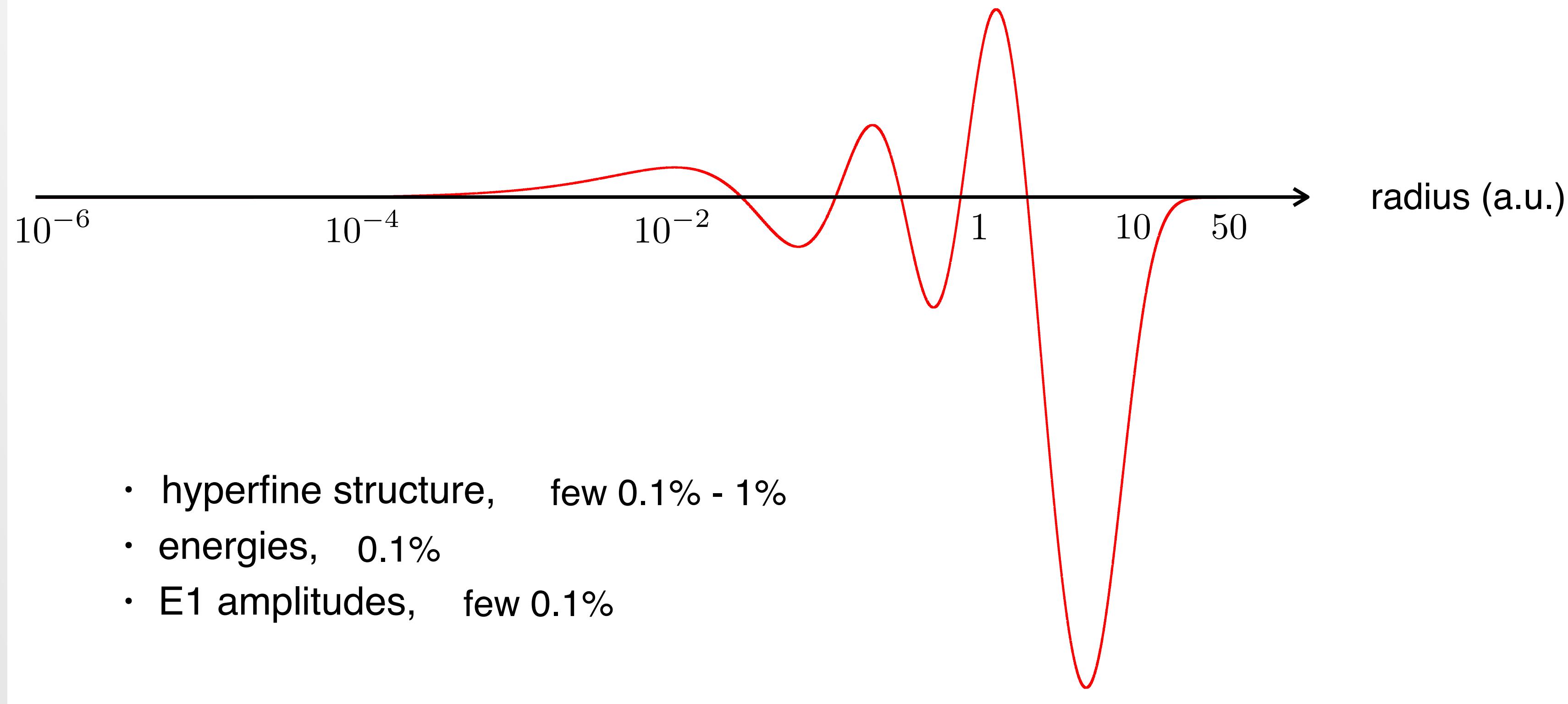
To maximise the discovery potential of precision atomic experiments

- Push state-of-the-art atomic calculations to 0.1% precision
 - Development of high-precision many-body methods
 - Improved benchmarking of atomic theory

Remove nuclear structure uncertainties that hinder tests of atomic theory

Benchmarking atomic theory

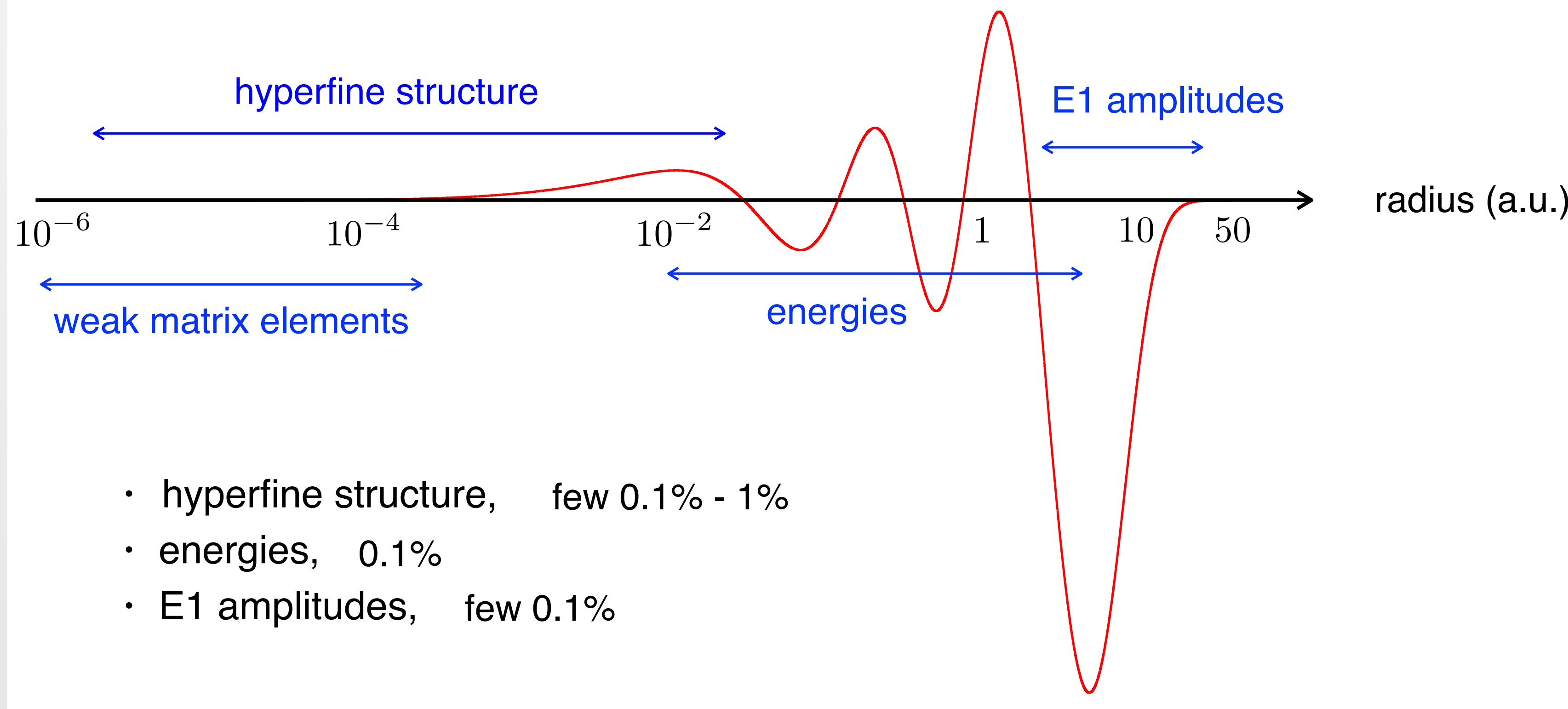
Upper radial component, Cs 6s:



$$E_{\text{PV}} = \sum_n \frac{\langle 7S_{1/2} | D | nP_{1/2} \rangle \langle nP_{1/2} | H_{\text{PV}} | 6S_{1/2} \rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \sum_n \frac{\langle 7S_{1/2} | H_{\text{PV}} | nP_{1/2} \rangle \langle nP_{1/2} | D | 6S_{1/2} \rangle}{E_{7S_{1/2}} - E_{nP_{1/2}}} = \xi Q_W$$

Benchmarking atomic theory

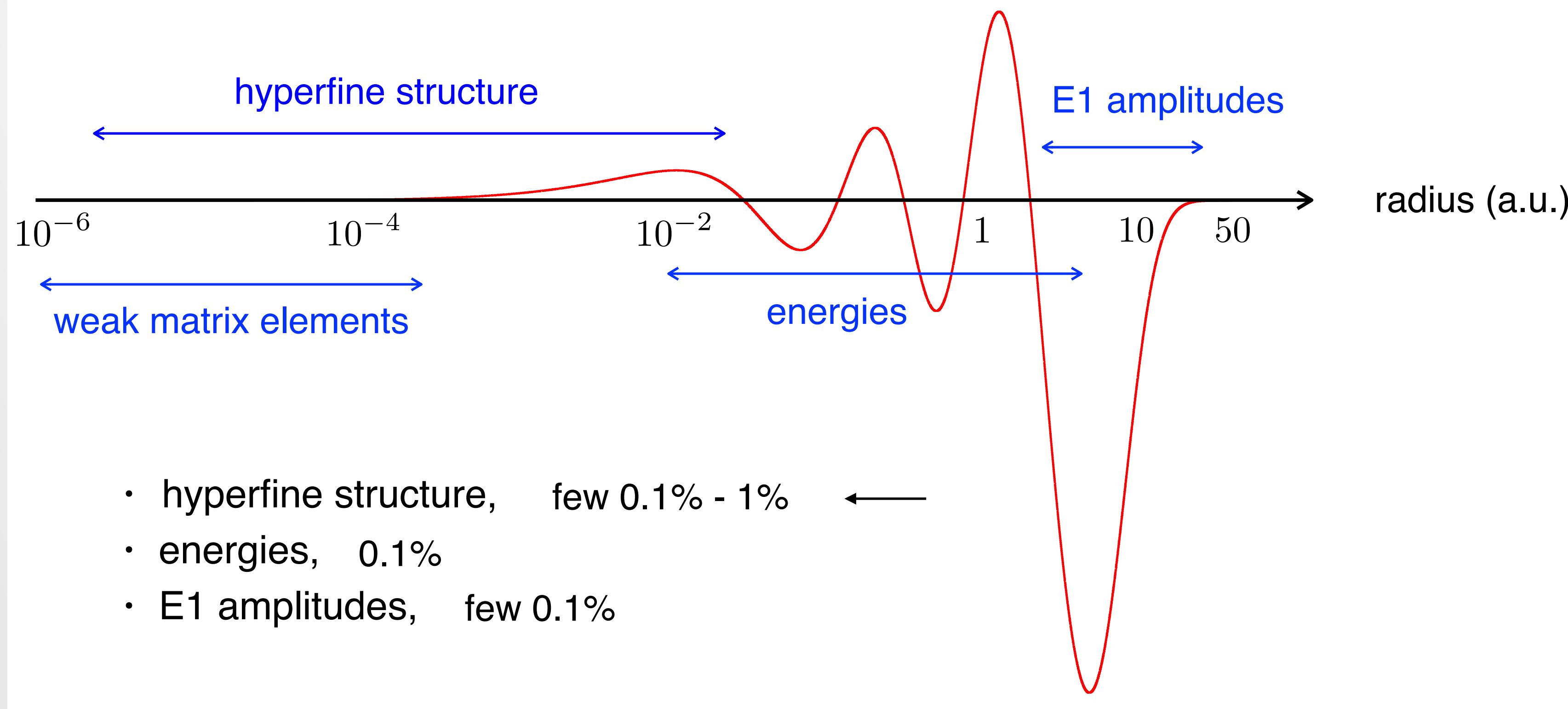
Upper radial component, Cs 6s:



$$E_{\text{PV}} = \sum_n \frac{\langle 7S_{1/2} | D | nP_{1/2} \rangle \langle nP_{1/2} | H_{\text{PV}} | 6S_{1/2} \rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \sum_n \frac{\langle 7S_{1/2} | H_{\text{PV}} | nP_{1/2} \rangle \langle nP_{1/2} | D | 6S_{1/2} \rangle}{E_{7S_{1/2}} - E_{nP_{1/2}}} = \xi Q_W$$

Benchmarking atomic theory

Upper radial component, Cs 6s:

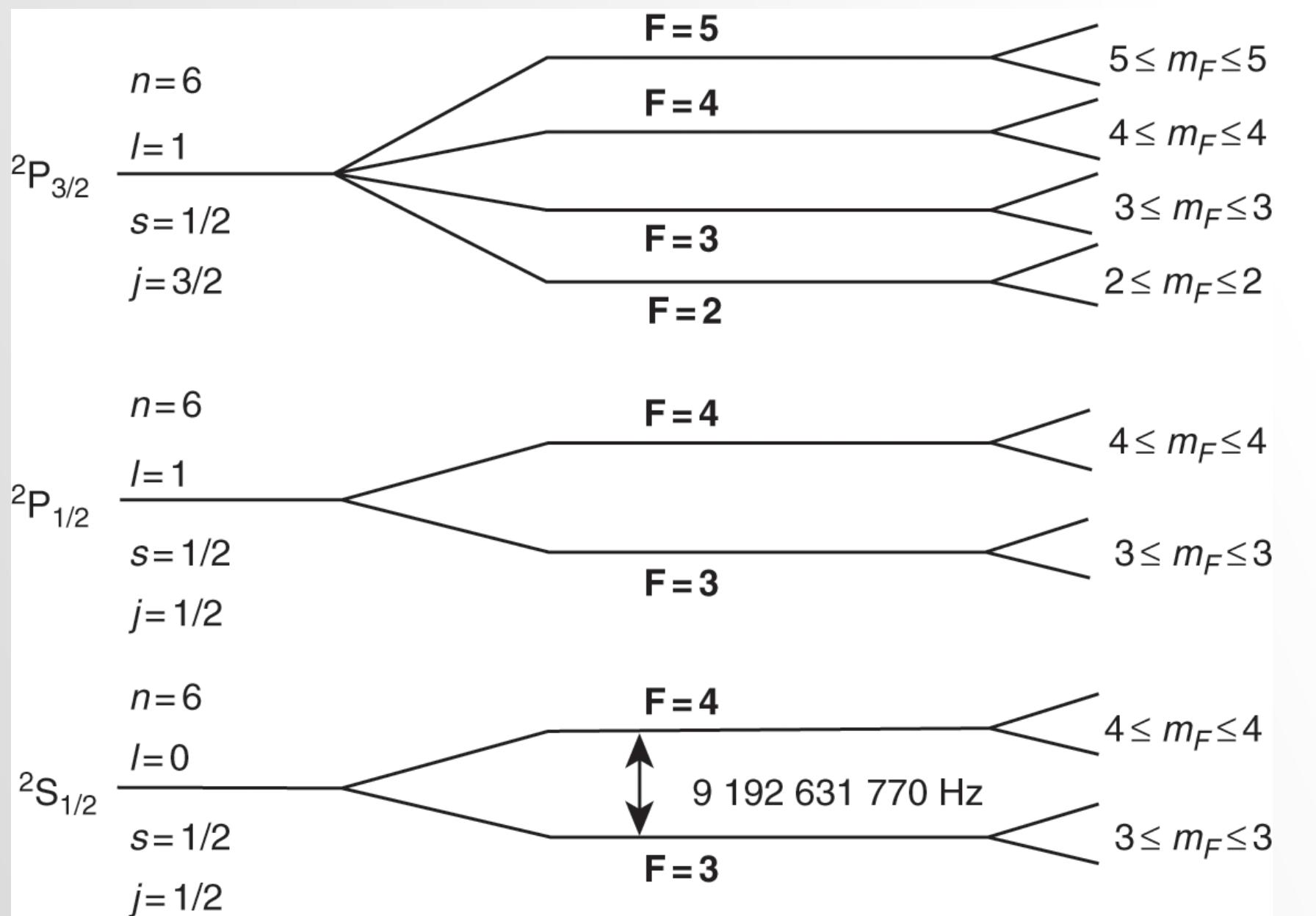


$$E_{\text{PV}} = \sum_n \frac{\langle 7S_{1/2} | D | nP_{1/2} \rangle \langle nP_{1/2} | H_{\text{PV}} | 6S_{1/2} \rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \sum_n \frac{\langle 7S_{1/2} | H_{\text{PV}} | nP_{1/2} \rangle \langle nP_{1/2} | D | 6S_{1/2} \rangle}{E_{7S_{1/2}} - E_{nP_{1/2}}} = \xi Q_W$$

Fine and hyperfine structure

Fine and hyperfine splitting of levels in ^{133}Cs

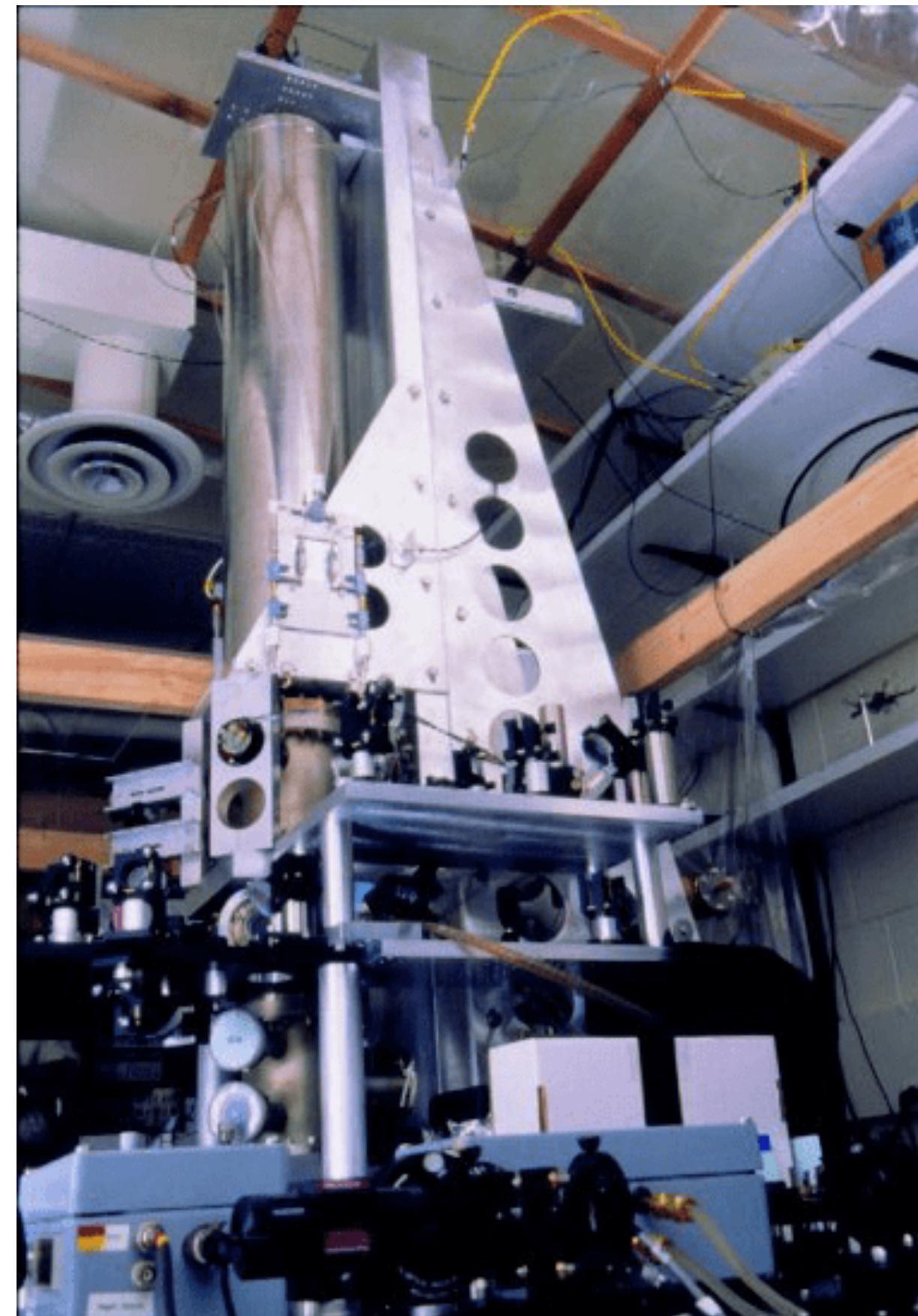
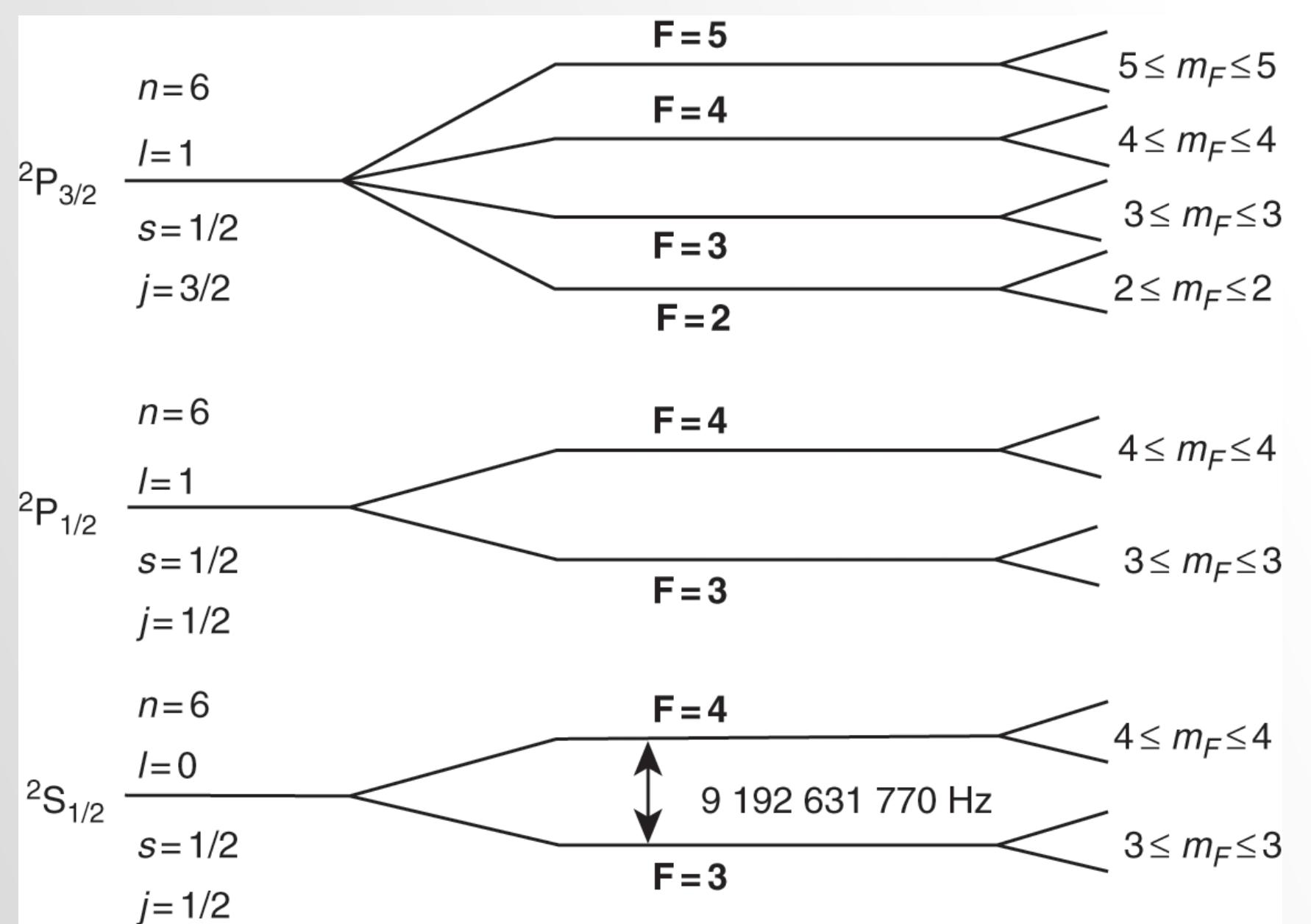
Nuclear spin $I = (7/2)^+$,
total angular momentum $\mathbf{F} = \mathbf{I} + \mathbf{J}$



Fine and hyperfine structure

Fine and hyperfine splitting of levels in ^{133}Cs

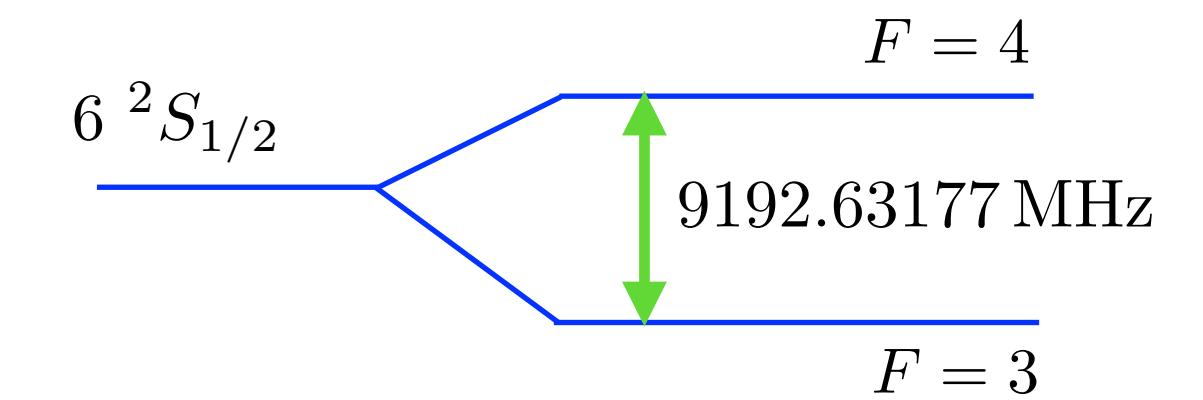
Nuclear spin $I = (7/2)^+$,
total angular momentum $\mathbf{F} = \mathbf{I} + \mathbf{J}$



NIST-F2 Atomic clock

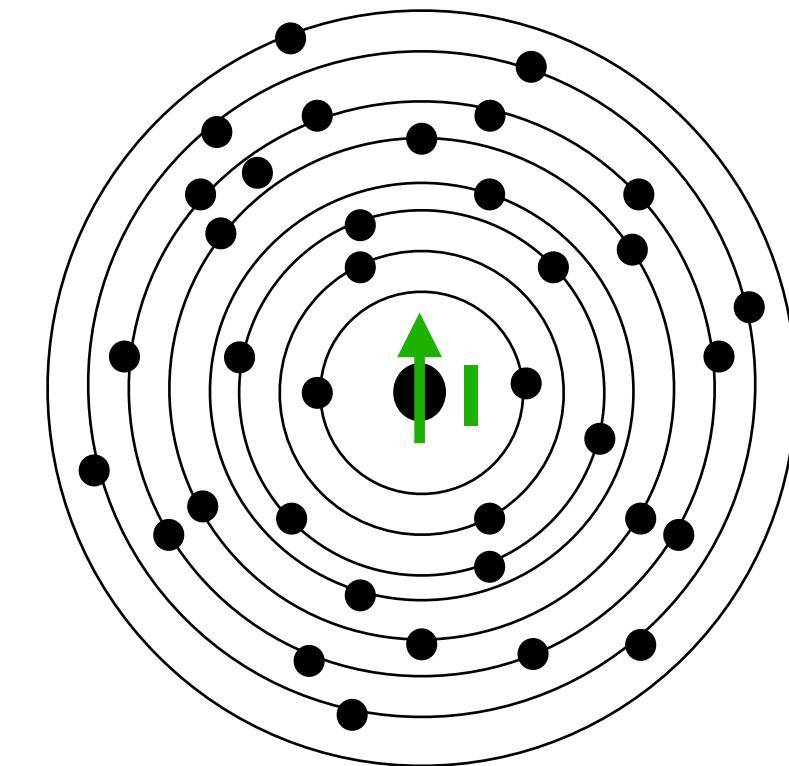
Primary standard for the SI
unit for time, the second

Hyperfine splitting in cesium

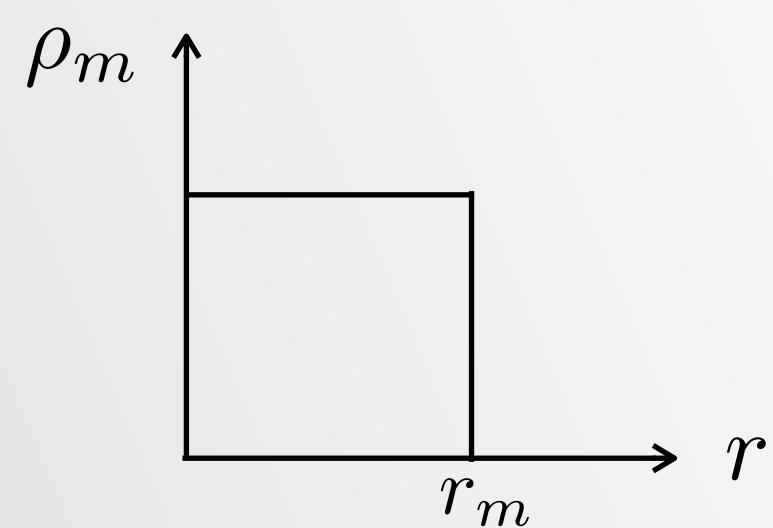


Modeling the hyperfine structure

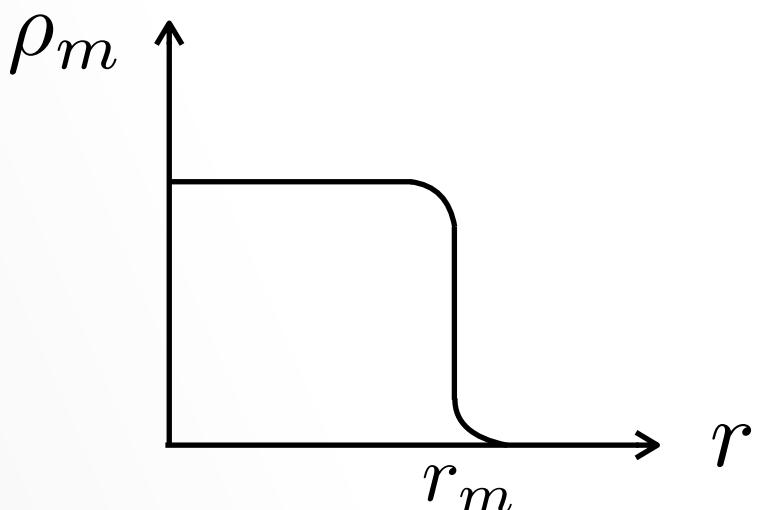
Interaction $h_{\text{hfs}} = \frac{1}{c} \frac{\mu \cdot (\mathbf{r} \times \boldsymbol{\alpha})}{r^3} F(r)$



Ball, $F(r) = (r/r_m)^3$



Fermi distribution



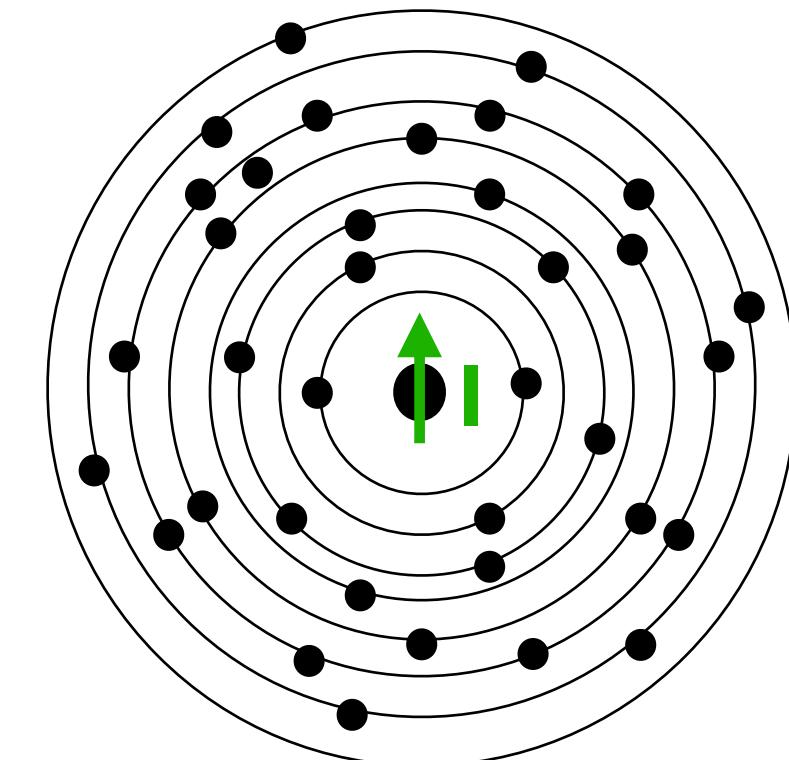
Standard ways to model
 $F(r)$, until recently

Hyperfine splitting quantified by hyperfine constant A , $A = A_0(1 + \epsilon) + \delta A^{\text{QED}}$

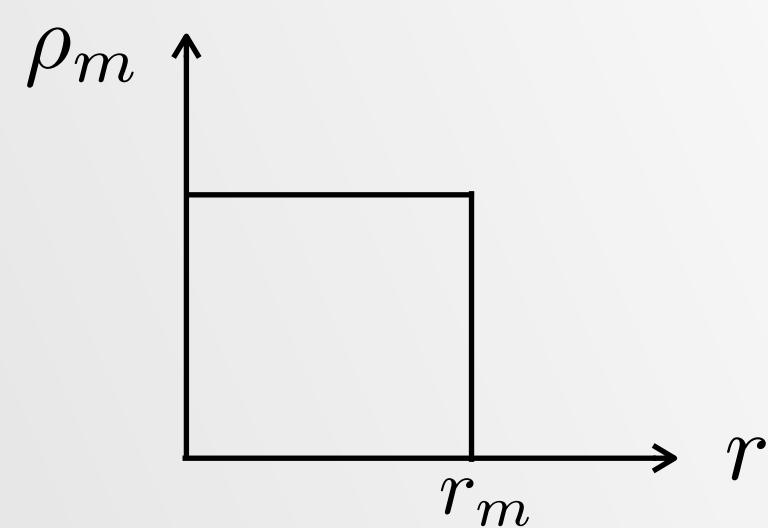
Modeling the hyperfine structure

nuclear magnetic moment $\mu = \mu\mathbf{I}/I$

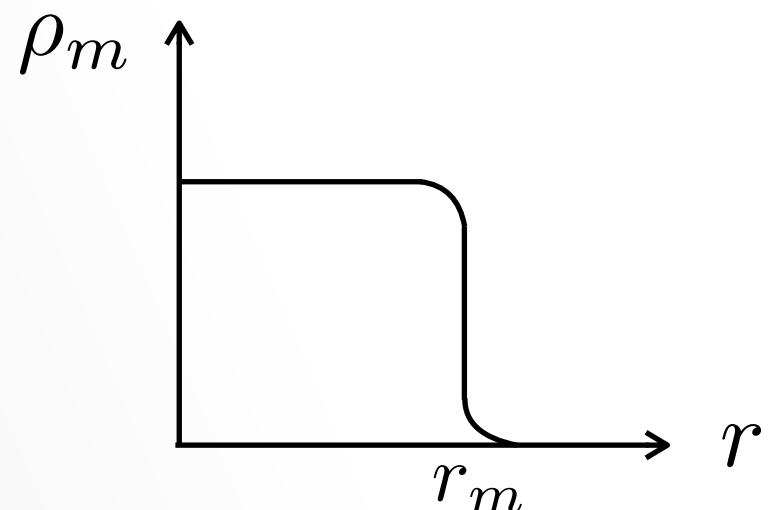
Interaction $h_{\text{hfs}} = \frac{1}{c} \frac{\mu \cdot (\mathbf{r} \times \boldsymbol{\alpha})}{r^3} F(r)$



Ball, $F(r) = (r/r_m)^3$



Fermi distribution



Standard ways to model
 $F(r)$, until recently

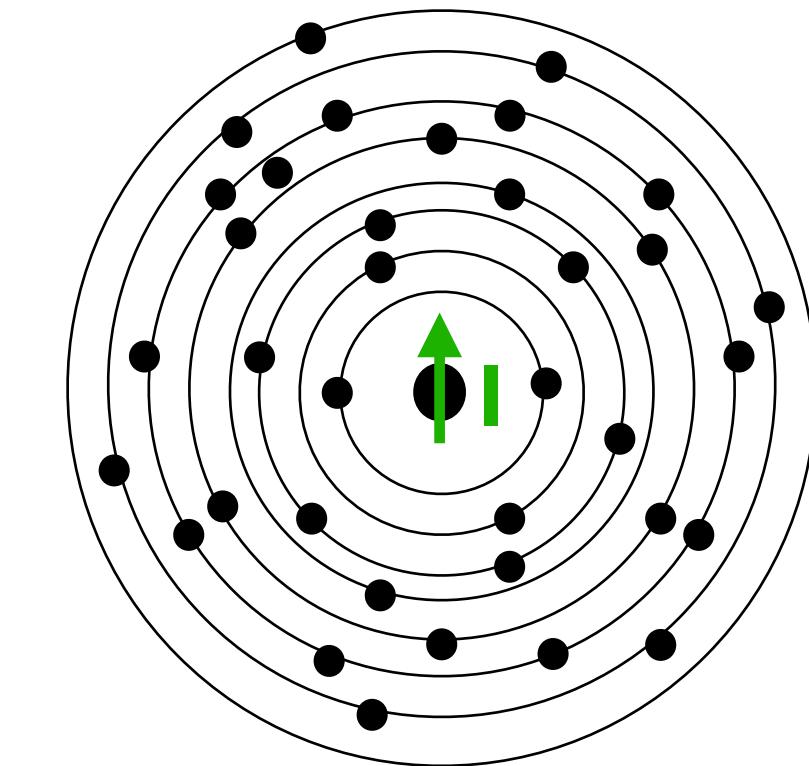
Hyperfine splitting quantified by hyperfine constant A , $A = A_0(1 + \epsilon) + \delta A^{\text{QED}}$

Modeling the hyperfine structure

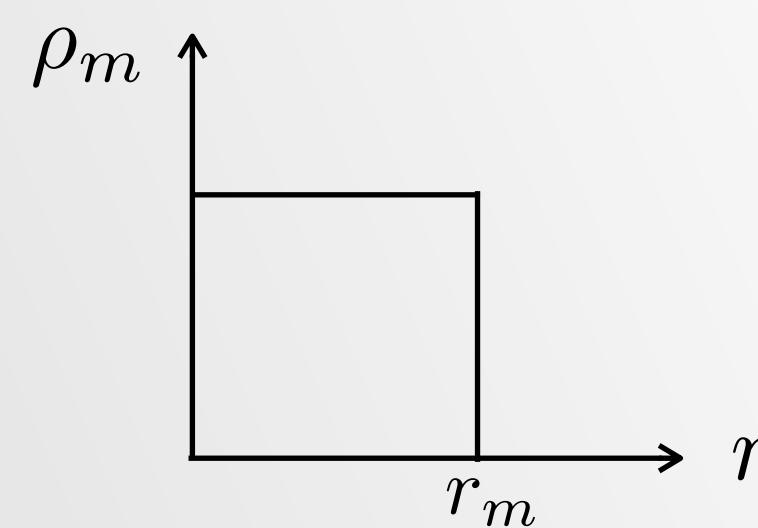
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Interaction $h_{\text{hfs}} = \frac{1}{c} \frac{\mu \cdot (\mathbf{r} \times \boldsymbol{\alpha})}{r^3} F(r)$

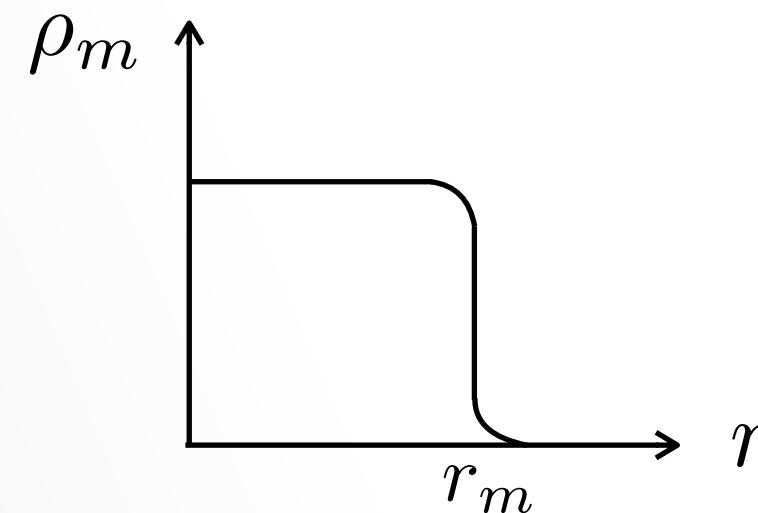
describes radial distribution of μ ;
point-nucleus, $F(r) = 1$



Ball, $F(r) = (r/r_m)^3$



Fermi distribution



Standard ways to model
 $F(r)$, until recently

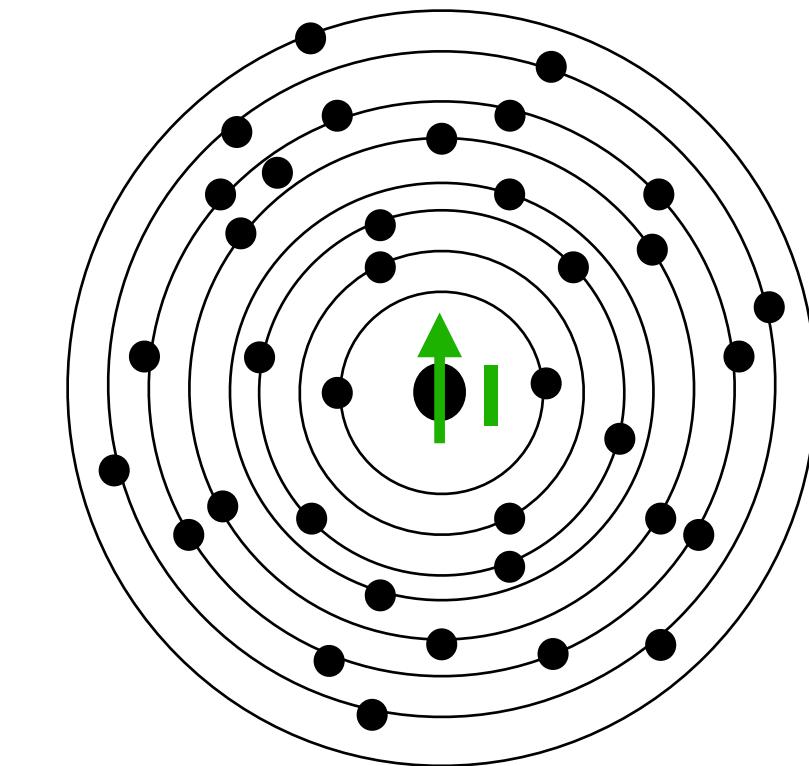
Hyperfine splitting quantified by hyperfine constant A , $A = A_0(1 + \epsilon) + \delta A^{\text{QED}}$

Modeling the hyperfine structure

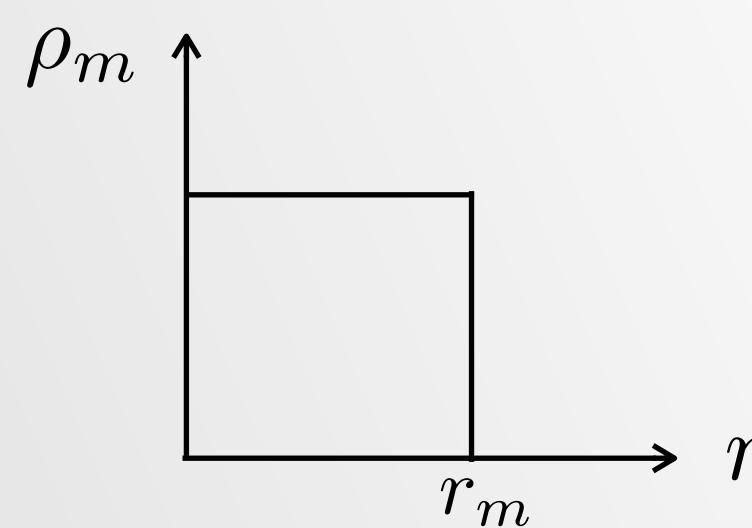
nuclear magnetic moment $\mu = \mu\mathbf{I}/I$

Interaction $h_{\text{hfs}} = \frac{1}{c} \frac{\mu \cdot (\mathbf{r} \times \boldsymbol{\alpha})}{r^3} F(r)$

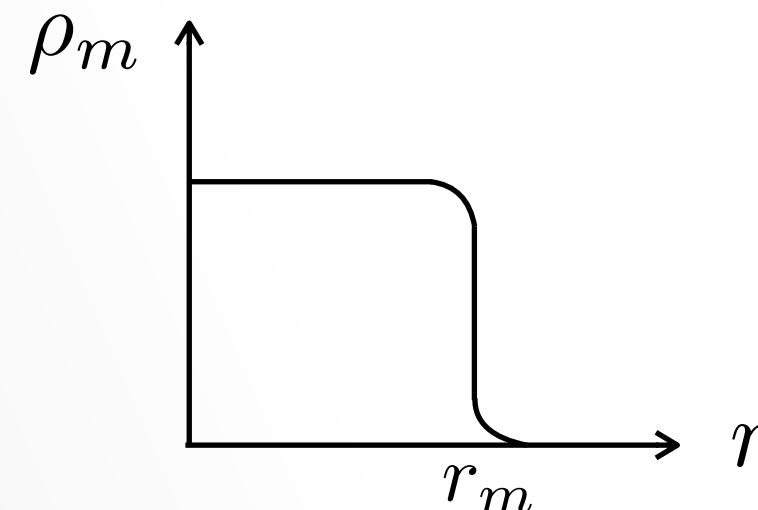
describes radial distribution of μ ;
point-nucleus, $F(r) = 1$



Ball, $F(r) = (r/r_m)^3$



Fermi distribution



Standard ways to model
 $F(r)$, until recently

Hyperfine splitting quantified by hyperfine constant A , $A = A_0(1 + \epsilon) + \delta A^{\text{QED}}$

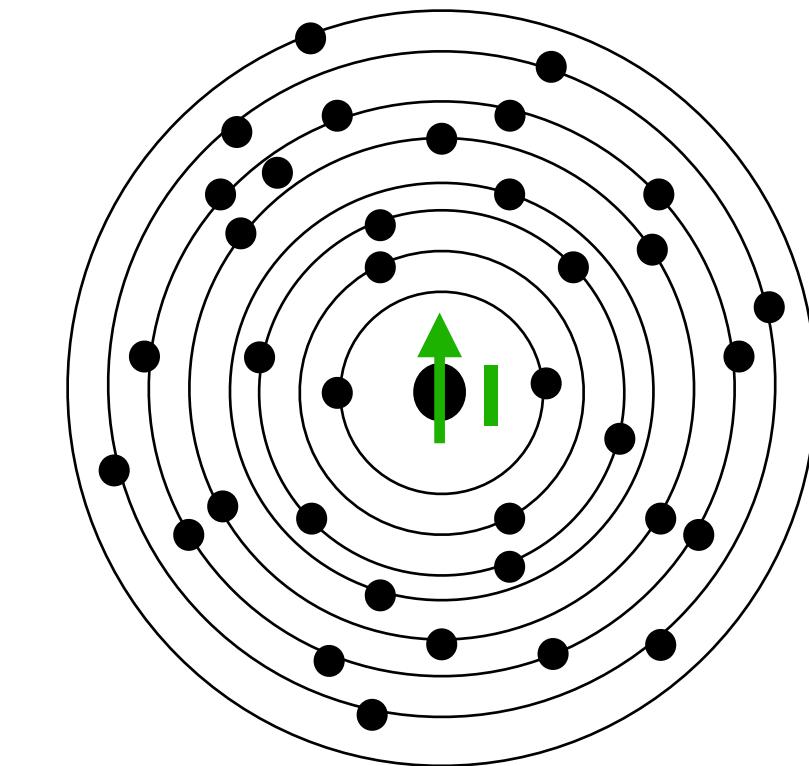
↑
Many-body result,
finite nuclear charge effect included

Modeling the hyperfine structure

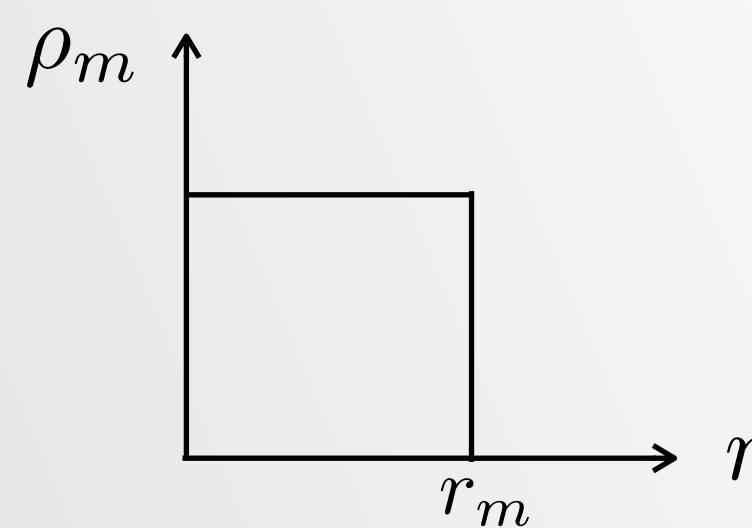
nuclear magnetic moment $\mu = \mu\mathbf{I}/I$

Interaction $h_{\text{hfs}} = \frac{1}{c} \frac{\mu \cdot (\mathbf{r} \times \boldsymbol{\alpha})}{r^3} F(r)$

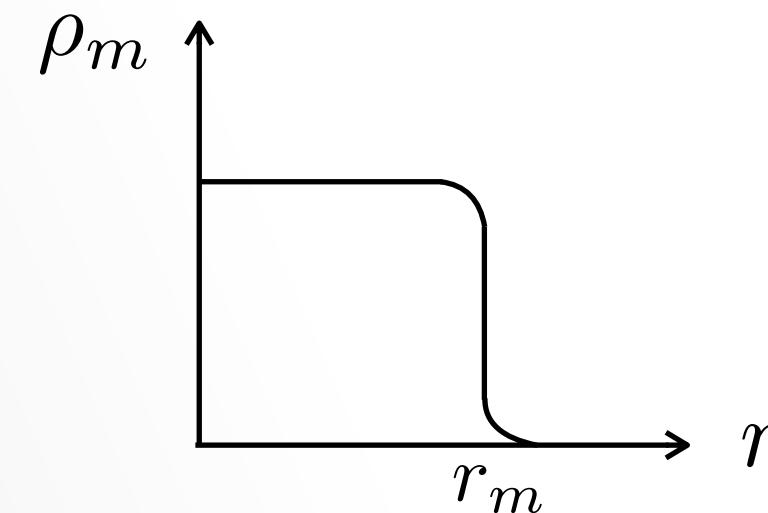
describes radial distribution of μ ;
point-nucleus, $F(r) = 1$



Ball, $F(r) = (r/r_m)^3$



Fermi distribution



Standard ways to model
 $F(r)$, until recently

Hyperfine splitting quantified by hyperfine constant A , $A = A_0(1 + \epsilon) + \delta A^{\text{QED}}$

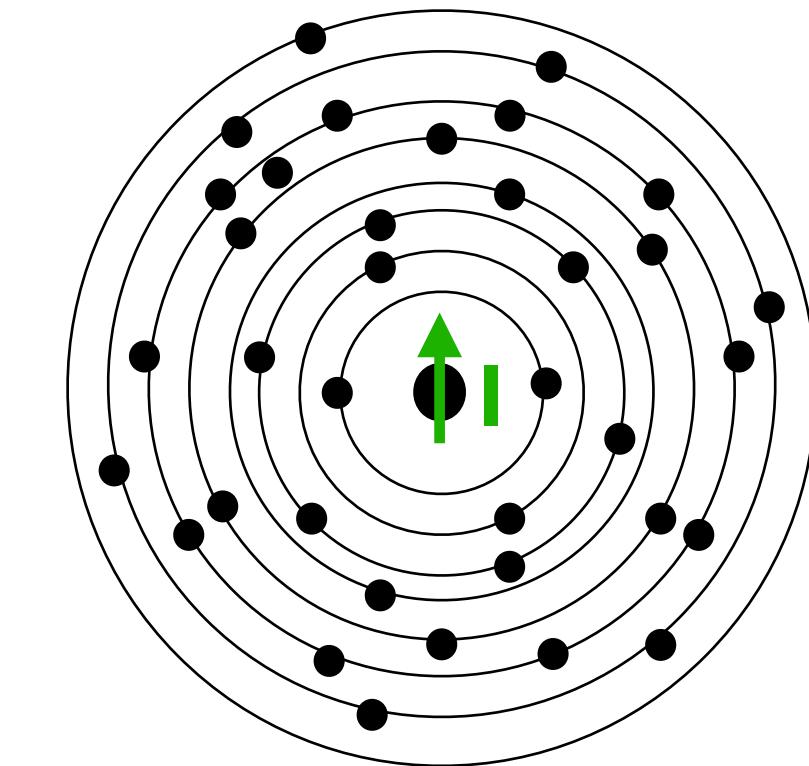
Bohr-Weisskopf (BW) effect or *magnetic hyperfine anomaly*
— finite nuclear magnetisation contribution

Modeling the hyperfine structure

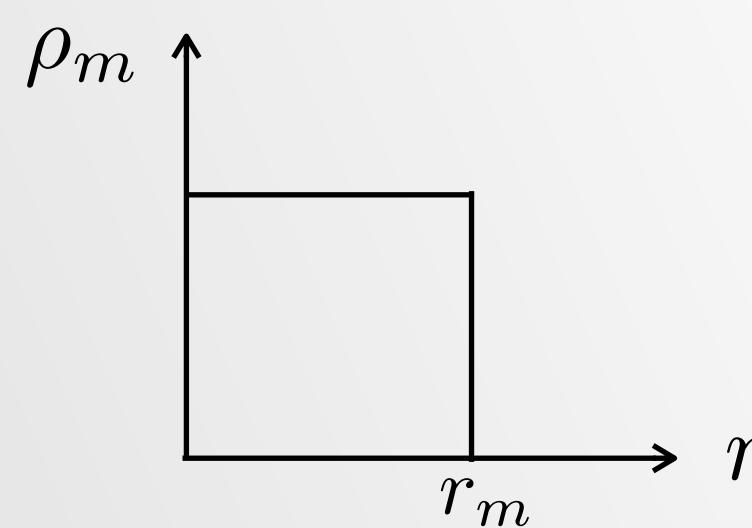
nuclear magnetic moment $\mu = \mu\mathbf{I}/I$

Interaction $h_{\text{hfs}} = -\frac{1}{c} \frac{\mu \cdot (\mathbf{r} \times \boldsymbol{\alpha})}{r^3} F(r)$

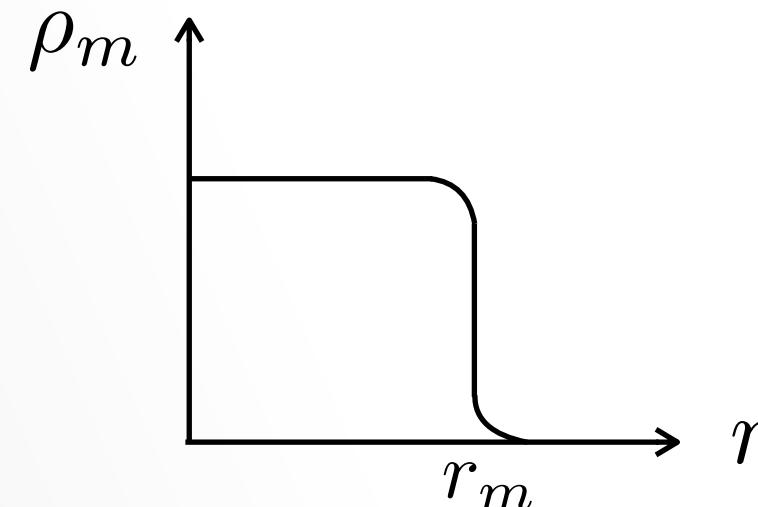
describes radial distribution of μ ;
point-nucleus, $F(r) = 1$



Ball, $F(r) = (r/r_m)^3$



Fermi distribution



Standard ways to model
 $F(r)$, until recently

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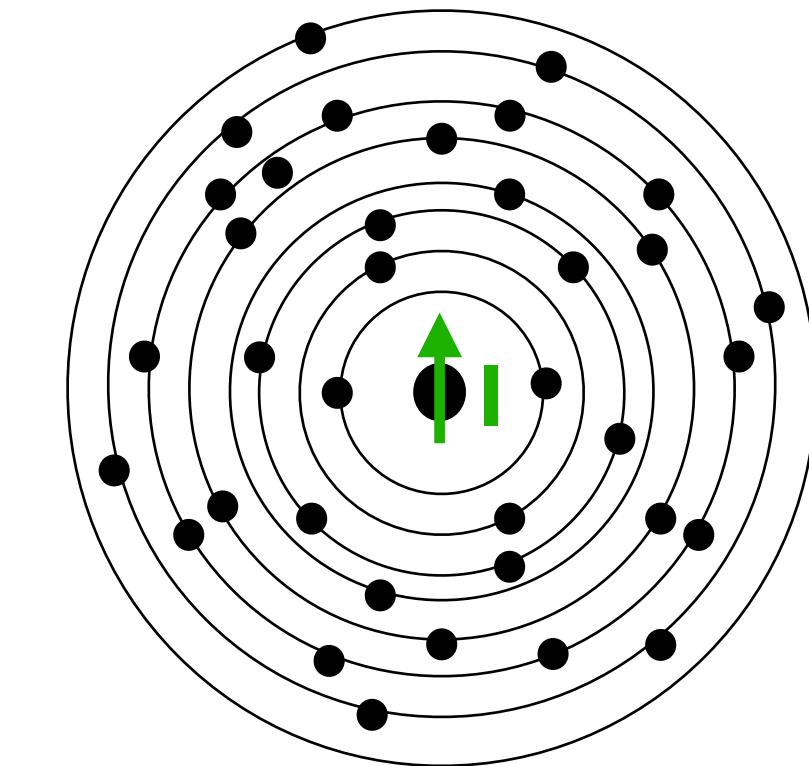
Quantum electrodynamics
radiative correction

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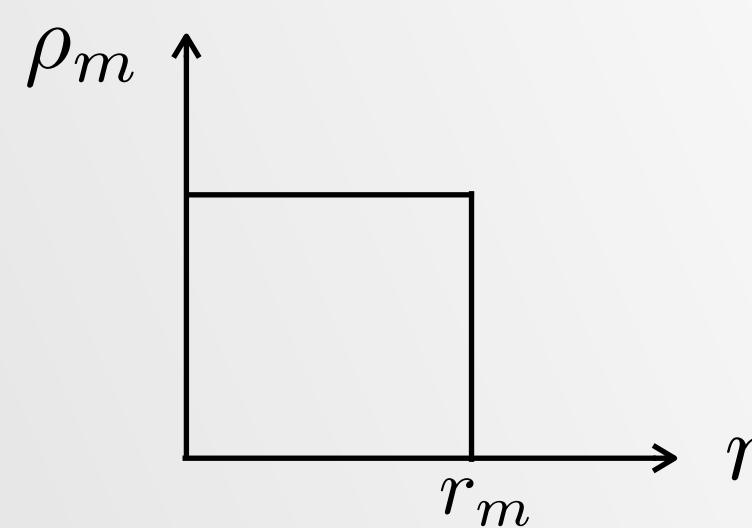
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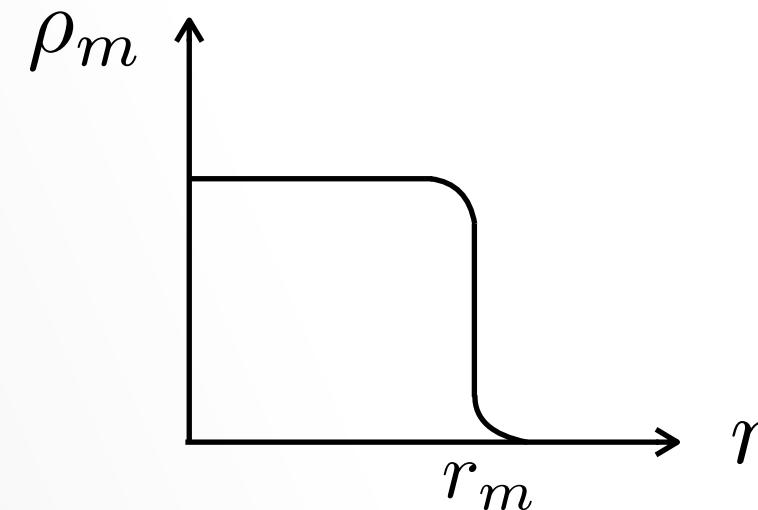
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contains factor μ

Hyperfine comparisons

$$A^{\text{expt}} \longleftrightarrow A_0(1 + \epsilon) + \delta A^{\text{QED}}$$

Provides test of atomic many-body theory in the nuclear vicinity *only if* the following properties/contributions are known well (< 0.1% uncertainty):

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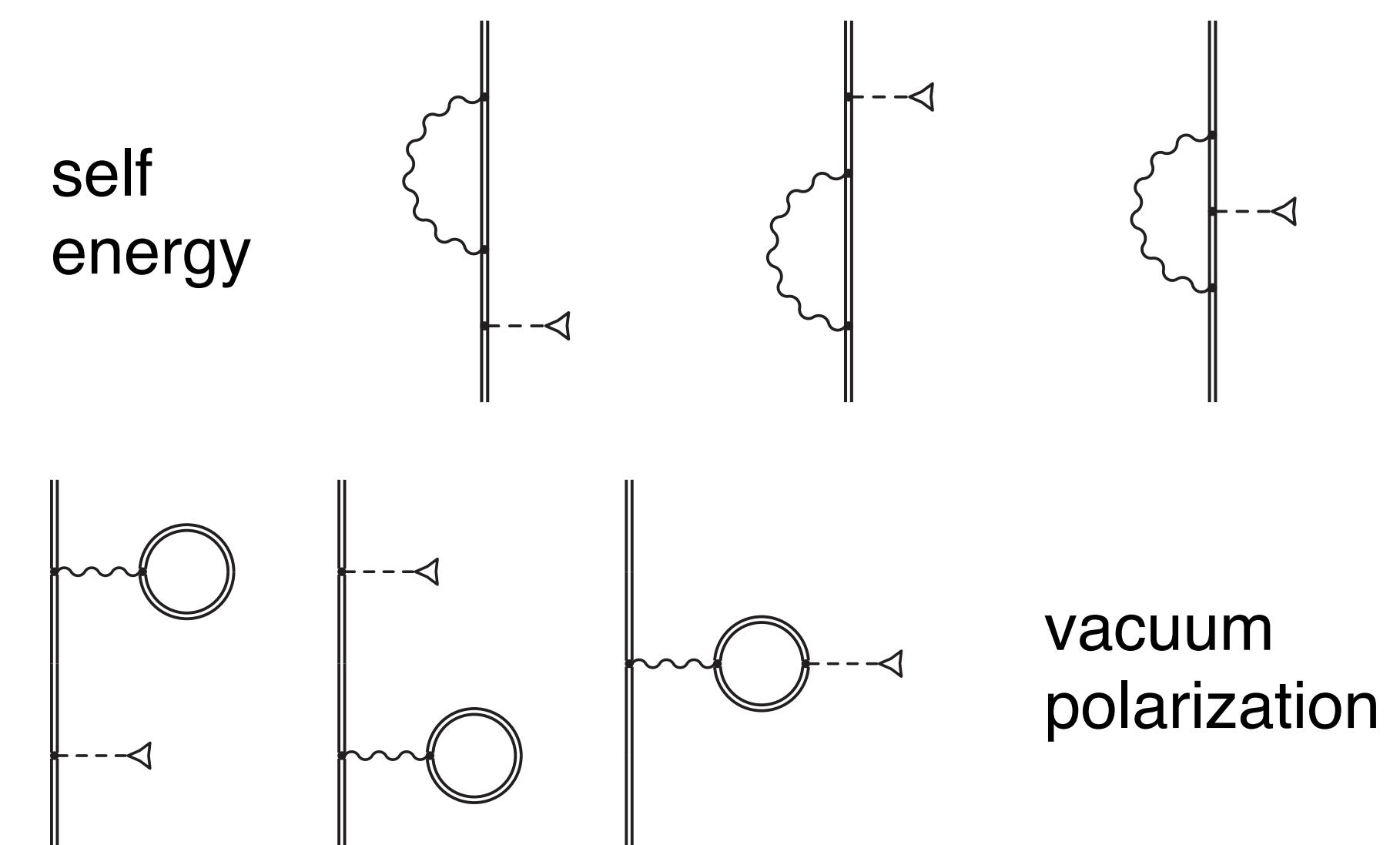
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QED corrections to g.s. hyperfine constants (%)

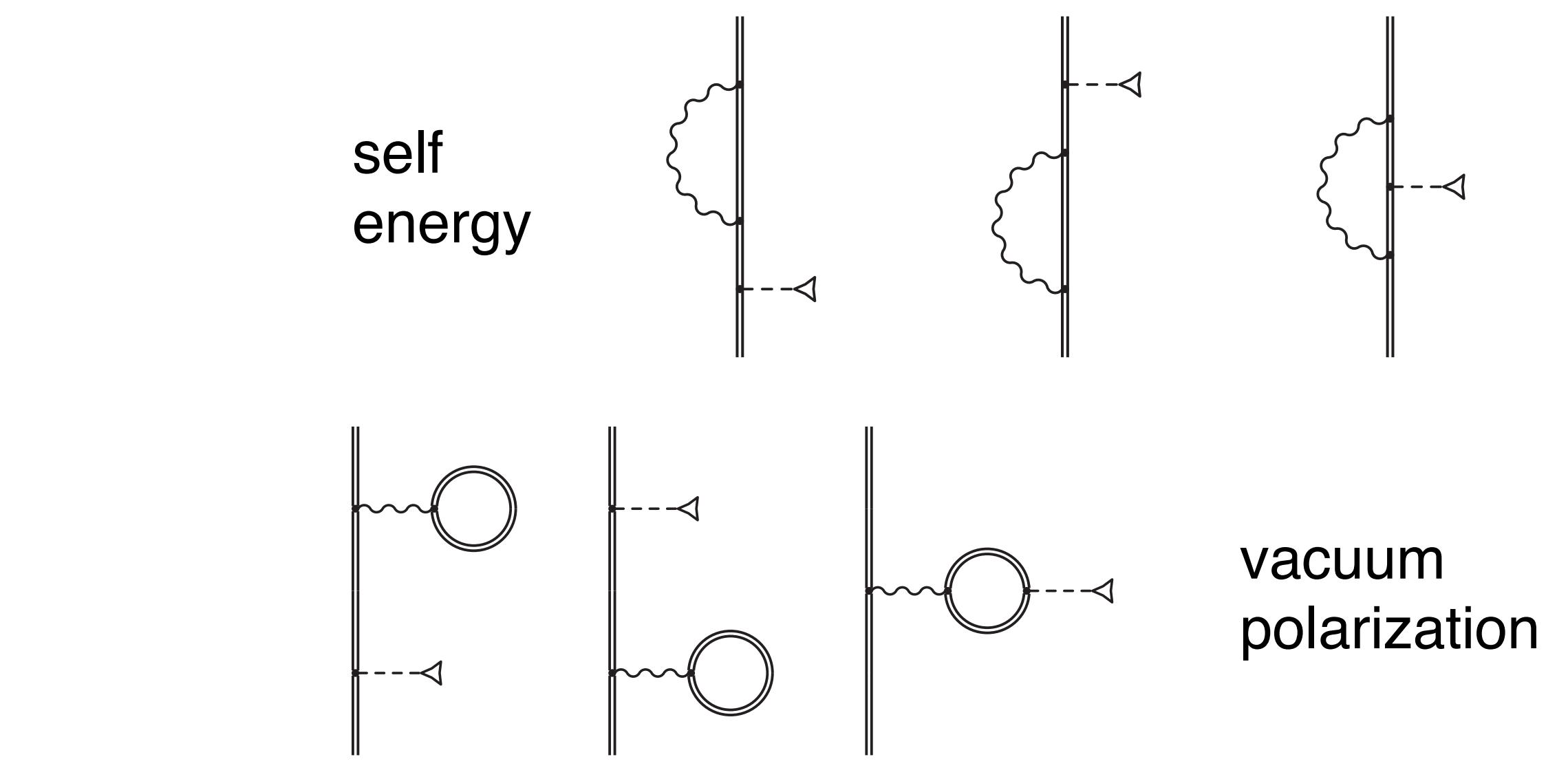
| Cs | Ba ⁺ | Fr | Ra ⁺ | Reference |
|----------|-----------------|----------|-----------------|--|
| -0.38(6) | -0.37(4) | -0.60(1) | -0.55(8) | Ginges, Volotka, Fritzsche, PRA (2017) |
| -0.42 | | -0.6 | | Sapirstein and Cheng, PRA (2003) |

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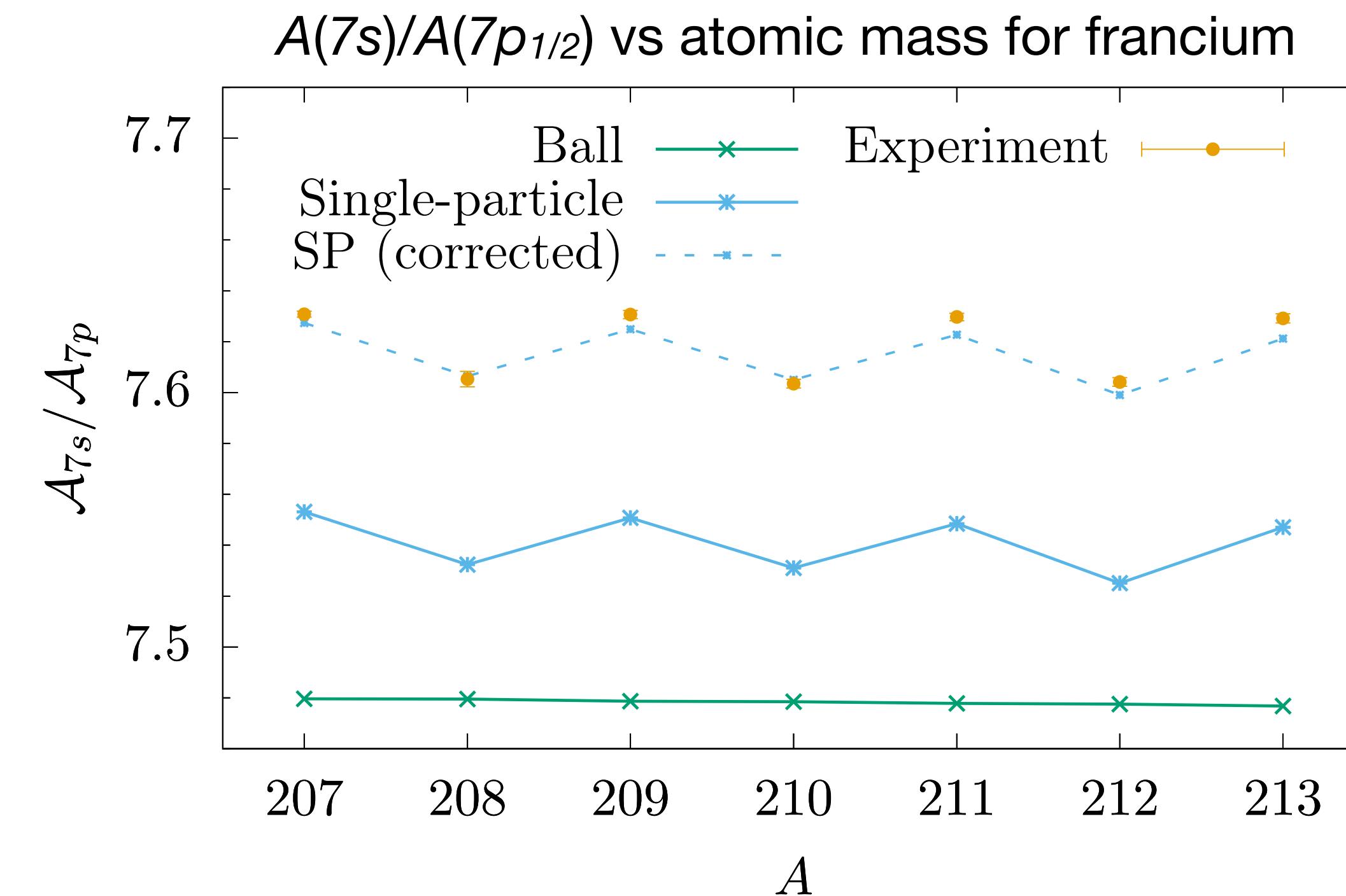
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Known with 1-2% uncertainty for Fr isotopes.
We can do better!

$$A^{\text{expt}} \longleftrightarrow A^{\text{th}}(\mu_{\text{th}})(\mu/\mu_{\text{th}})$$

Found μ with 0.5% uncertainty



Roberts and Ginges, PRL (2020)

Experimental values: FrPNC collaboration

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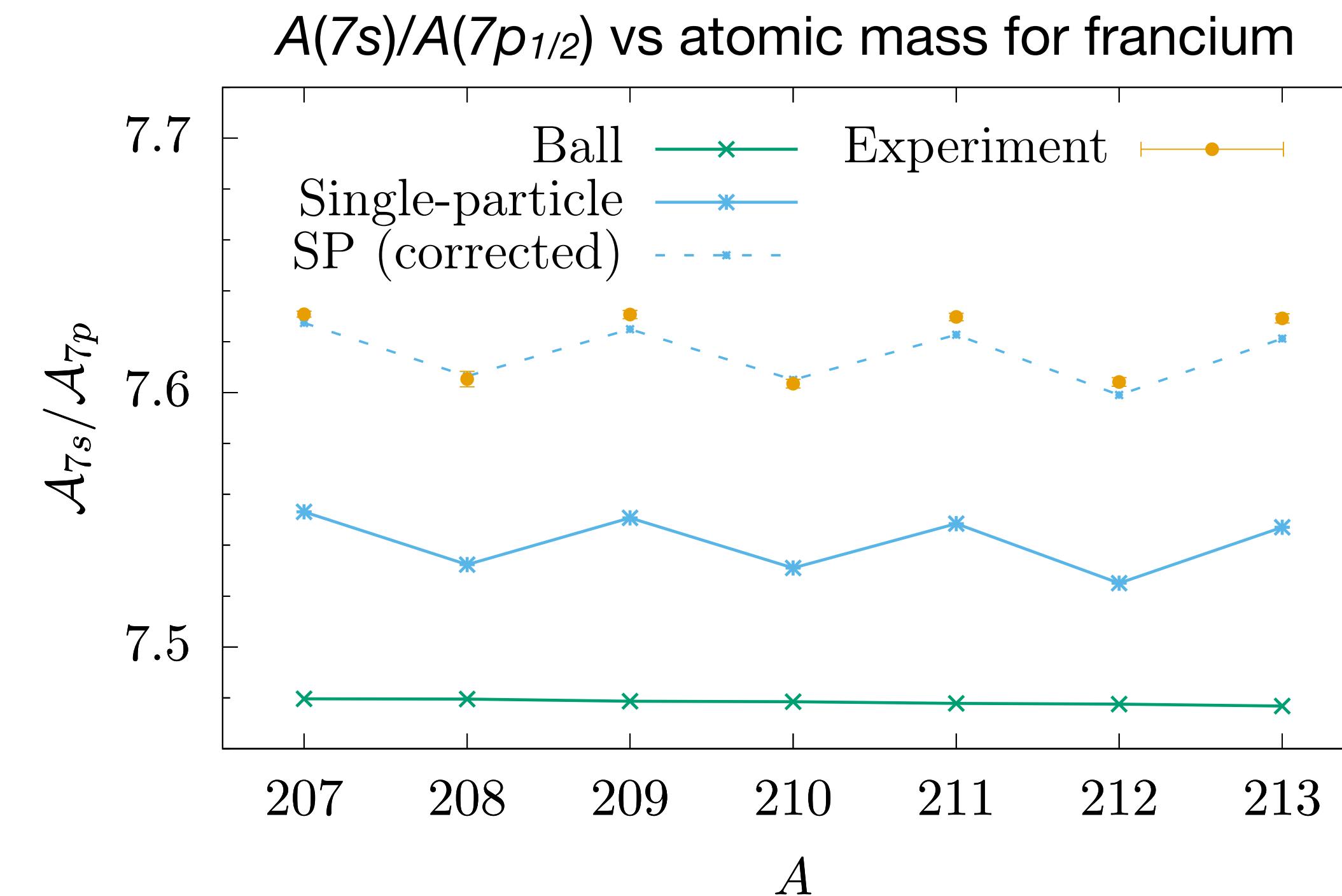
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SP model:

$$F(r) = \left(\frac{r}{r_m}\right)^3 \left[1 - 3 \ln\left(\frac{r}{r_m}\right) \frac{\mu_N}{\mu} \left(-\frac{2I-1}{8(I+1)} g_S + \frac{2I-1}{2} g_L \right) \right]$$

for $I=L+1/2$

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BW corrections (%) to hyperfine constants

| nuclear model | ^{133}Cs | $^{135}\text{Ba}^+$ | ^{211}Fr | $^{225}\text{Ra}^+$ |
|----------------------|-------------------|---------------------|-------------------|---------------------|
| ball | -0.71 | -0.74 | -2.7 | -2.8 |
| single-particle (SP) | -0.21 | -1.0 | -1.3 | -2.8 |
| SP (WS, spin-orbit) | -0.19(14) | -1.3(4) | -1.4(5) | -4.3(13) |

Difference

0.5%

1.3%

Hyperfine comparisons

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Total hyperfine intervals

Calculations of hyperfine intervals and comparison with experiment. Units: MHz

| | ^{133}Cs | $^{135}\text{Ba}^+$ | ^{211}Fr | $^{225}\text{Ra}^+$ |
|----------------|-------------------|---------------------|-------------------|---------------------|
| Many-body | 9229.5 | 7286.8 | 45374 | -29113 |
| BW | -17.0(131) | -91.8(275) | -641(244) | 1267(380) |
| QED | -35.1(58) | -27.1(30) | -273(56) | 159(23) |
| Total theory | 9177.4 | 7167.9 | 44460 | -27687 |
| Experiment | 9192.6 | 7183.3 | 43570 | -27731 |
| Difference | -15.2 | -15.4 | 890 | 44 |
| Difference (%) | -0.17(16) | -0.21(38) | 2.0(6)(20) | -0.2(14) |

Ginges, Volotka, Fritzsche, PRA (2017)

Extraction of Ra^+ BW effect, -4.7%:

And from molecules! RaF

Skripnikov, J. Chem. Phys. (2020)

S. Wilkins et al., arxiv:2311.04121

Differential hyperfine anomaly

Ratio of hyperfine constants of different isotopes of same element:

$$\mathcal{A}^{(1)}/\mathcal{A}^{(2)} = g_I^{(1)}/g_I^{(2)}(1 + {}^1\Delta^2)$$

Typically for nuclei of different spin: ${}^1\Delta^2 \approx \epsilon^{(1)} - \epsilon^{(2)}$

→ Gives *difference* in BW effect for different isotopes

| | | Isotope 1 | | | | Isotope 2 | | | | Differential anomaly ${}^1\Delta^2$ (%) | | |
|----------------------|------------|-----------|---------|-------------------------------|-----------------------------|-----------|---------|-------------------------------|-----------------------------|---|--------|-----------------------|
| | | A | I^π | $\epsilon_{\text{Ball}} (\%)$ | $\epsilon_{\text{SP}} (\%)$ | A | I^π | $\epsilon_{\text{Ball}} (\%)$ | $\epsilon_{\text{SP}} (\%)$ | Ball | SP | Expt. [59] |
| ${}^{37}\text{Rb}$ | $5s_{1/2}$ | 85 | $5/2^-$ | -0.306 | 0.044 | 87 | $3/2^-$ | -0.306 | -0.278 | -0.001 | 0.323 | 0.35142(30) |
| | | | | | | 86 | 2^- | -0.306 | -0.139 | 0.000 | 0.183 | 0.17(9) |
| ${}^{47}\text{Ag}$ | $5s_{1/2}$ | 107 | $1/2^-$ | -0.497 | -4.20 | 103 | $7/2^+$ | -0.493 | -0.347 | -0.018 | -3.88 | -3.4(17) |
| | | | | | | 109 | $1/2^-$ | -0.498 | -3.78 | 0.007 | -0.431 | -0.41274(29) |
| ${}^{55}\text{Cs}$ | $6s_{1/2}$ | 133 | $7/2^+$ | -0.716 | -0.209 | 131 | $5/2^+$ | -0.716 | -0.596 | -0.001 | 0.389 | 0.45(5) ^a |
| | | | | | | 135 | $7/2^+$ | -0.716 | -0.247 | 0.002 | 0.039 | 0.037(9) ^b |
| | | | | | | 134 | 4^+ | -0.716 | -0.371 | 0.000 | 0.163 | 0.169(30) |
| ${}^{56}\text{Ba}^+$ | $6s_{1/2}$ | 135 | $3/2^+$ | -0.747 | -1.03 | 137 | $3/2^+$ | -0.747 | -1.03 | 0.001 | 0.001 | -0.191(5) |

Roberts and Ginges, PRA (2021)

Expt. data from: Persson, At. Data Nucl. Data Tables (2013)

BW effect – properties

Relative BW correction

$$\epsilon = \frac{\int_0^{r_m} dr f(r) g(r) [F(r) - 1] / r^2}{\int_0^{\infty} dr f(r) g(r) / r^2}$$

Shabaev et al., PRL (2001)
Skripnikov, J. Chem. Phys. (2020)
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- In the nuclear region, the electrons see the unscreened Coulomb field of the nucleus
- Since the binding energies $\varepsilon \ll V(r)$, wave functions with the same angular dependence are proportional.

$$\begin{bmatrix} V(r) - \varepsilon & c(\kappa/r - \partial_r) \\ c(\kappa/r + \partial_r) & V(r) - \varepsilon - 2c^2 \end{bmatrix} \begin{bmatrix} f_{n\kappa} \\ g_{n\kappa} \end{bmatrix} = 0$$

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BW effect is independent of principal quantum number!

$$\Rightarrow \epsilon_{n\kappa} = \epsilon_{n'\kappa}$$

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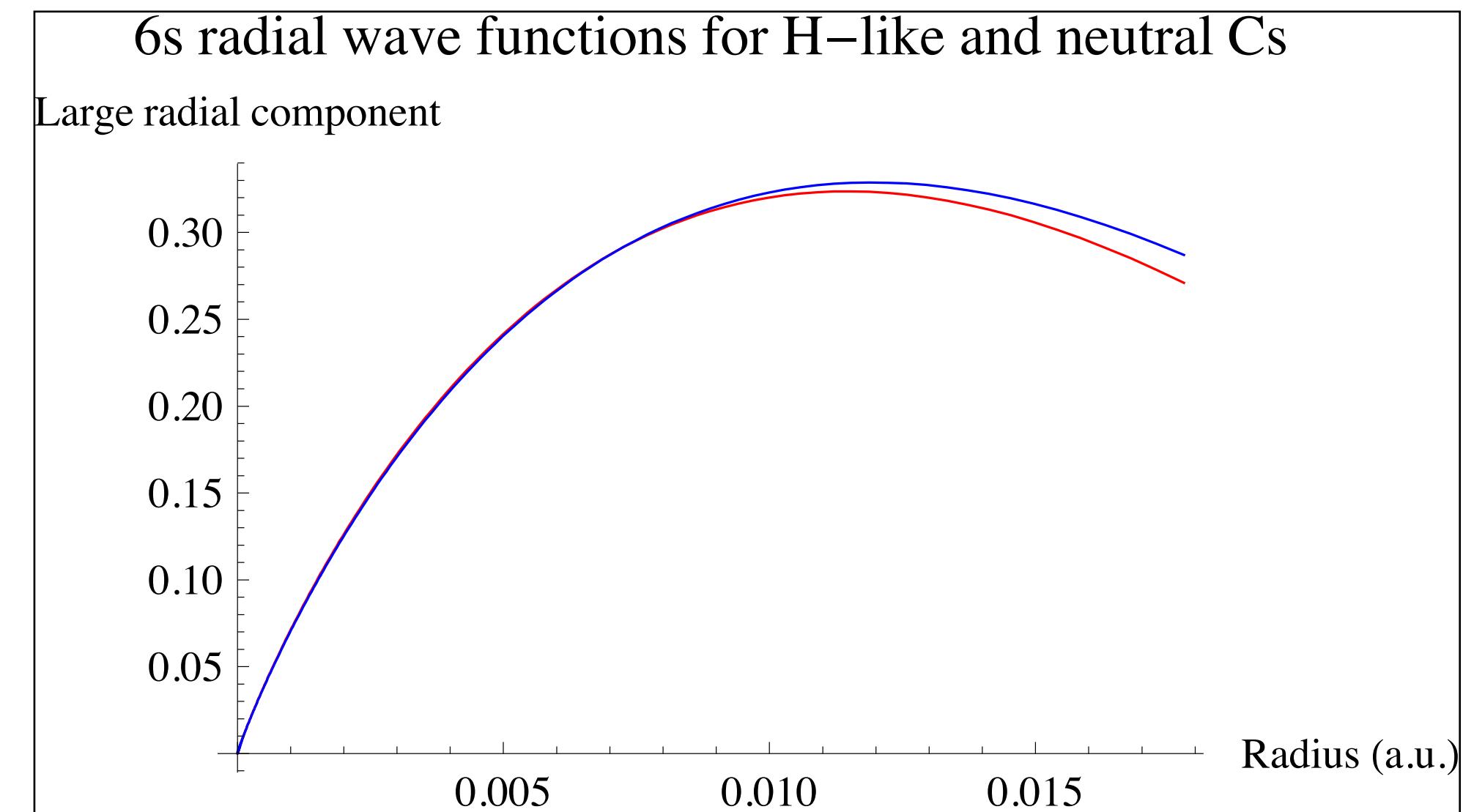
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Also, in the nuclear region, for heavy systems:

$$f_{s_{1/2}} \propto g_{p_{1/2}} , \quad g_{s_{1/2}} \propto f_{p_{1/2}}$$

BW effects in atoms related to BW matrix element
for 1s state of H-like ion

Shabaev et al., PRL (2001)
Skripnikov, J. Chem. Phys. (2020)
Roberts, Ranclaud, Ginges, PRA (2022)

BW effect: ratio method

By taking a ratio of two states with different principal quantum number, dependence on BW effect may be removed!

$$A_{n\kappa}^{\text{th}} = A_{0,n\kappa} \left(A_{n'\kappa}^{\text{exp}} / A_{0,n'\kappa} \right)$$

May be used to make high-precision predictions of the hyperfine constants!

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From Quirk et al., PRA (2022)
[Dan Elliott group, Purdue]

| State | A _{hfs} (MHz) | | | |
|-------|------------------------|-----------------|-----------|-----------|
| | Experiment | Theory | Ref. [37] | Ref. [16] |
| 12s | 26.318 (15) | 26.31 (10) [24] | 26.28 | 26.30 (2) |
| 13s | 18.431 (10) | 18.40 (11) [25] | | 18.42 (1) |

Ref. [16] : Grunefeld, Roberts, Ginges, PRA (2019)

from Quirk et al., PRA (2023)
[Dan Elliott group, Purdue]

| A _{hfs} (MHz) for 8p _{1/2} | |
|--|---|
| A | Source |
| Experiment | |
| 42.97 (10) | Tai <i>et al.</i> , 1973 [40] |
| 42.92 (25) | Cataliotti <i>et al.</i> , 1996 [48] |
| 42.95 (25) | Liu & Baird, 2000 [49] |
| 42.933 (8) | This work |
| Theory | |
| 42.43 | Safronova <i>et al.</i> , 1999 [46] |
| 42.32 | Tang <i>et al.</i> , 2019 [47] |
| 42.95 (9) | fit method, Grunefeld <i>et al.</i> , 2019 [34] |
| 42.93 (7) | ratio method, Grunefeld <i>et al.</i> , 2019 [34] |

Ratio method: Ginges and Volotka, PRA (2018)

BW effect: from H-like ion

$$\mathcal{A}_{\text{expt}}^{1s} = \mathcal{A}_0^{1s}(1 + \epsilon^{1s}) + \delta\mathcal{A}_{\text{QED}}^{1s}$$

BW effect with $\sim 1\%$ uncertainty from H-like ${}^{203,205}\text{TI}$,
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*H-like ion result may be used to find BW effect in
many-electron atoms!*

$$\mathcal{A} = \mathcal{A}_0(1 + x_{\text{scr}} \epsilon^{1s}) + \delta\mathcal{A}_{\text{QED}}$$

↑
electronic
screening factor

x_{scr} independent of the nuclear model!

s states: $x_{\text{scr}} \approx 1$, negligible uncertainty

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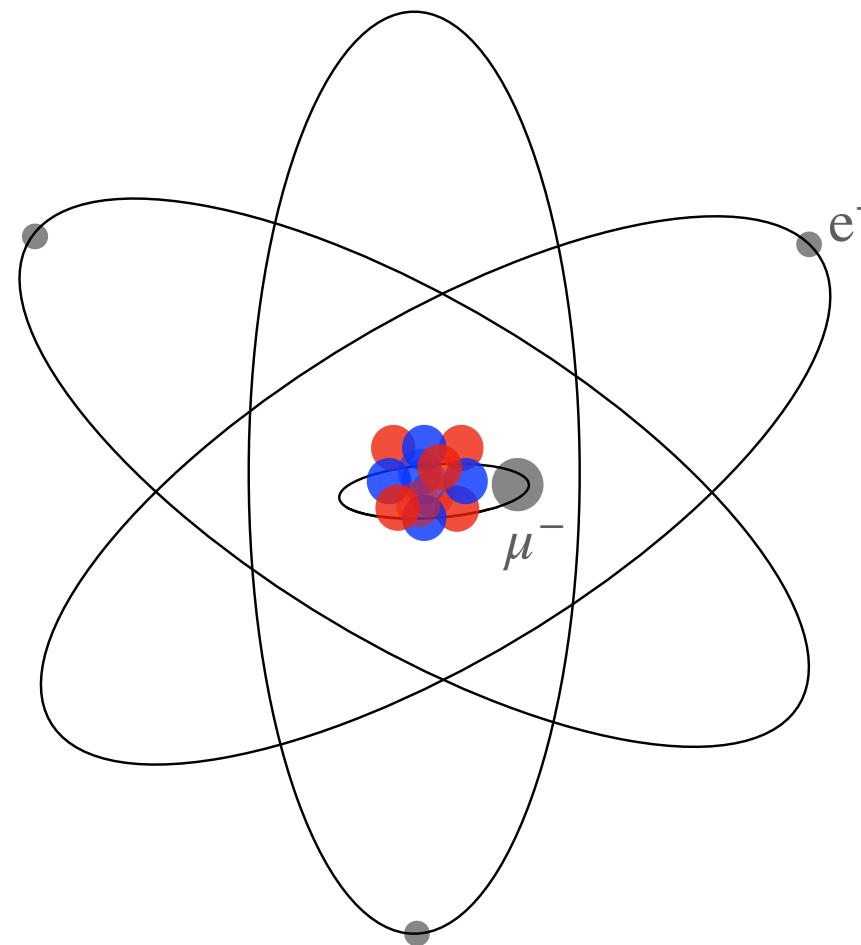
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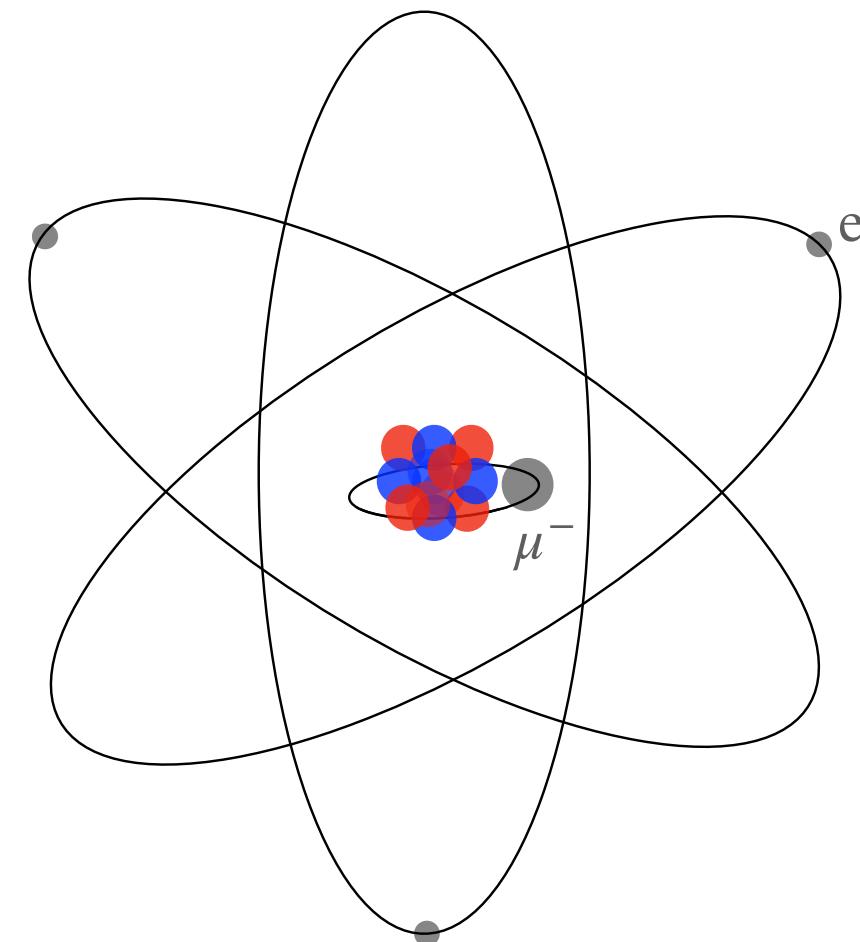
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Elizarov et al., Opt. Spectrosc. (2006)
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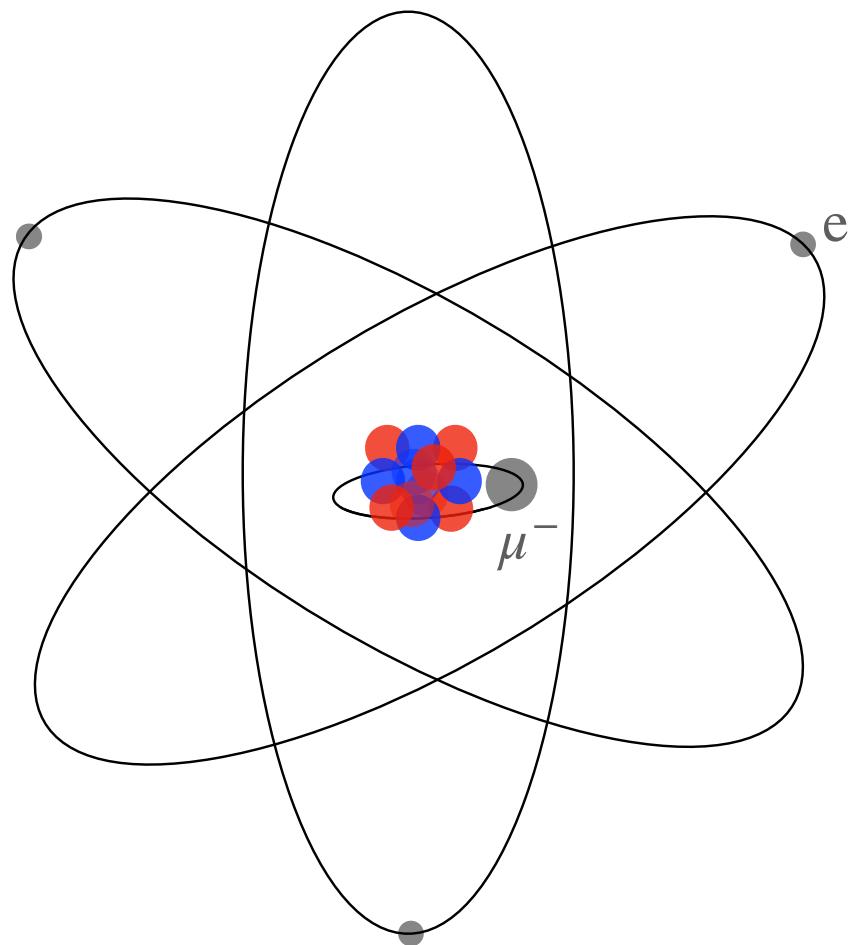
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“ball”/fermi model: -0.7%

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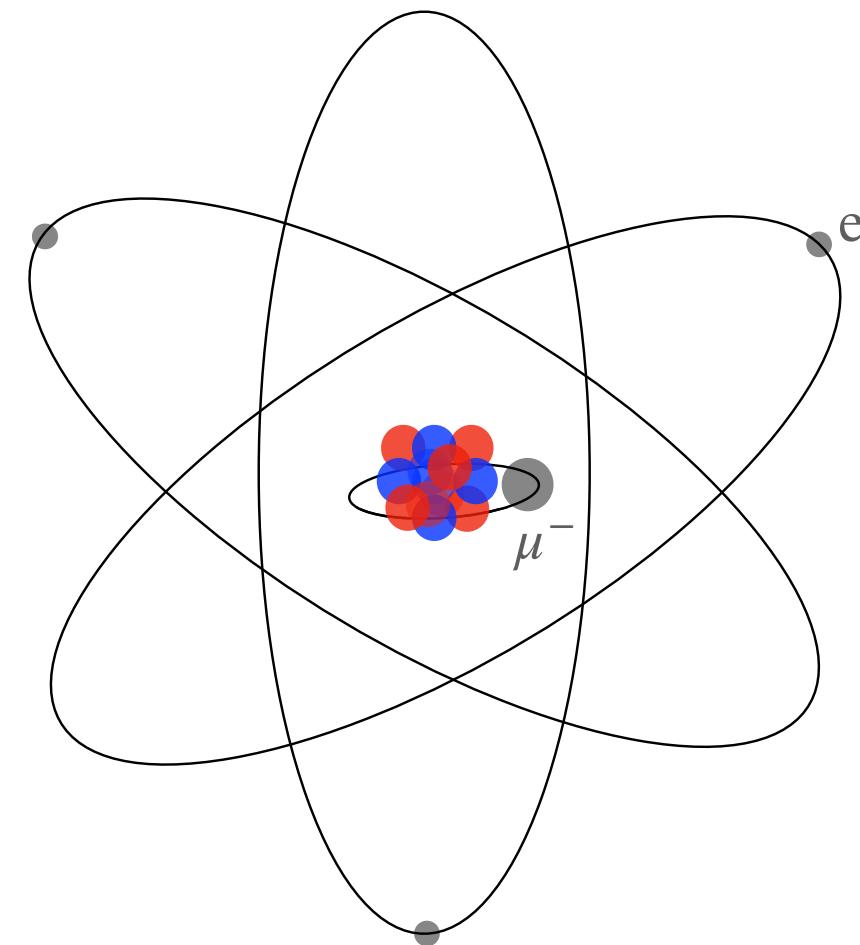
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Empirically-deduced BW effect ($-\epsilon$) in %

| | μ -atoms | | H-like ions | | Atoms |
|---------------------|--------------|-----------|-------------|-----------|-------|
| | μ exp | μ exp | H-like exp | μ exp | |
| ${}^{133}\text{Cs}$ | 18(14) | 0.23(17) | ... | 0.24(18) | |
| ${}^{203}\text{Tl}$ | 50.8(1.6) | 1.93(15) | 2.21(8) | | |
| ${}^{205}\text{Tl}$ | 51.8(8) | 1.98(15) | 2.25(8) | | |
| ${}^{209}\text{Bi}$ | 28.8(3.9) | 0.98(14) | 1.03(5) | | |

Bohr-Weisskopf effect summary

Accurate modelling of the finite magnetisation distribution in atomic nuclei is important for

- Hyperfine comparisons
 - Tests of atomic wave functions in the nuclear region
 - Reducing APV theory uncertainty to 0.1%
- Nuclear structure theory
- Determination of nuclear moments
- Probing the neutron distribution
- Tests of quantum electrodynamics

Summary

Atoms can be used to do breakthrough particle physics!

- Atomic parity violation
- Time-reversal-violating electric dipole moments

Lots of interdisciplinary discoveries that can be made on the way!

- Includes nuclear physics insights

Precision atomic theory

- Necessary and difficult! Though proceeding to reduce atomic theory uncertainties

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- Includes nuclear physics insights

Precision atomic theory

- Necessary and difficult! Though proceeding to reduce atomic theory uncertainties

Summary

Atoms can be used to do breakthrough particle physics!

- Atomic parity violation
- Time-reversal-violating electric dipole moments

Lots of interdisciplinary discoveries that can be made on the way!

- Includes nuclear physics insights

Precision atomic theory

- Necessary and difficult! Though proceeding to reduce atomic theory uncertainties

Thank you!

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